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# Black-box vs. White-box Models, Integrated vs. Cascade Simulations, and Multi-agent Simulation vs. Computational Fluid Dynamics

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**Abstract**: This article summarizes the concepts related to "simulation," originally introduced by John von Neumann and considered one of the most highly visible scientific terms today. Simulations aim to model complex dynamic systems in the real world, allowing us to predict their spatiotemporal structure. Modeling and simulation are required to control any dynamic system, which in turn enables us to maximize the resource output from a system while mitigating constraints to ensure its sustainability. Simulation covers a wide range of dynamic systems from white-box to black-box models, depending on the transparency of each system. A physical system can be modeled using a white-box model because the governing equations are already given. However, the dynamics of a human decision process, or a human entity itself, is hardly treated as transparent, which inevitably leads to a black-box model. Another key idea related to simulation is "coupling," which connects two or more different sub-dynamical systems using an integrated or cascade approach. One such important application is the merged technology of computational fluid dynamics and multi agent simulation. This paper presents concrete examples.

Keywords: Multi agent simulation (MAS); integrated and cascade simulations, black-box and white-box models

## 1. Introduction–The original meaning of "simulation"

The term "simulation" was first introduced by John von Neumann in the 1940s. Simulations facilitate the prediction of how systems will evolve over time in cases wherein a set of governing equations to globally describe a system's dynamics cannot be known but local rules to depict how each particle composing the system interacts with other surrounding particles can be known. Inspired by the Latin word simulates meaning "simulated," von Neumann called a bottom–up approach a "simulation" as opposed to a top–down approach. In line with this concept, von Neumann and Stanislaw Ulam solved the problem regarding the behaviors of neurons, which led them to conceptualize the Monte Carlo simulation, in which a set of local-event rules combined with the roulette wheel technique stochastically predicts the outcome of the entire sequence of events (i.e., the global dynamics)[1)]. This is what a multi agent simulation (MAS) is pursuing. In the 1990s, it became one of the Zeitgeist words coinciding with the outbreak of complex science and the astonishing progress of computing performance. Following von Neumann's definition, we should hesitate to call computational fluid dynamics (CFD) a simulation because the set of governing equations, known as the Navier–Stokes equations, is given to us. However, this article calls CFD simulation based on the current custom. In contrast, representative MAS models, such as pedestrian simulations based on the so-called *social force model* (e.g.[2)]) and a traffic flow model based on the *car-following* formulation (e.g.[3)]), should be regarded as exact simulations.

## 2. System rainbow: White-box vs. black-box model

The targets of modeling (i.e., what one intends to model) might vary even if they are limited to the building physics sphere. In the 1970s, Karplus[4)] provided the spectrum of mathematical modeling, which was called "System Rainbow," as shown in Fig. 1. All aspects to be explored during modeling are categorized somewhere between a "white-box model" and a "black-box model."

With white-box modeling, we can expect to precisely predict the dynamics of a system because an established mathematical model can transparently capture the internal structure of the system, thus allowing for accurate forecasting of what actually happens in the time direction. Electrical and chemical systems are classified as white-box models. A superior white-box model allows the control, design, and optimization of a system because the dynamics are fully supported by physics formulations. In contrast, human social systems are considered black-box models. Therefore, we must rely on a certain statistical model to analyze a cause–effect relationship, which we cannot deterministically predict but must statistically infer a predicted result. For example, when dealing with a psychological system, we cannot help but rely on a fully black-box model that only describes an input–output relation. In such a case, the system can no longer be an "objective" for control to obtain preferable results; it is simply a "target" for rough estimation.

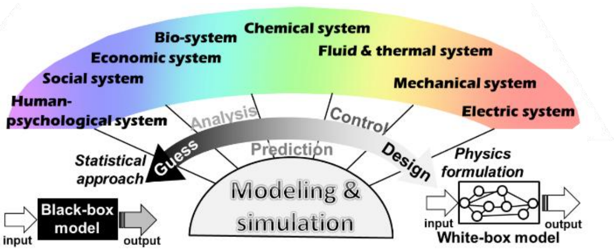



**Fig. 1:** Black-box and white-box models mapped in the proposed System Rainbow Karplus[4]. A human system encompassing human decision-making processes at various stages is represented by a black-box model. In contrast, a physical system can be formulated by a set of governing equations explicitly depicting the dynamics. This is called the white-box model.

Yet, numerous studies on artificial intelligence (AI) issues over the last couple of decades have altered the picture depicted above. The artificial neural network, which is based on Frank Rosenblatt's "perceptron"[5] emulates how a human brain stores the knowledge obtained from human experiences and draws an output to classify complex problems (e.g.[6]). This makes the modeling of the human decision-making process more in line with what an actual human does, thus moving away from the black-box model approach. In addition, reinforcement learning (e.g.[7]), combined with deep learning (e.g.[8]), which is technically supported by super computation with parallel processing, expands the possibility of modeling the dynamics of the human decision-making process. In fact, one of the prominent topics in the field of evolutionary game theory is the MAS model, which reproduces two coexisting agents: human agents emulated by either game theory or prospect theory or by other conventional ideas and "bot" agents equipped with AI. Such an MAS model, for example, aims to explore the social dilemma structure in the cyber–real worlds we are currently facing (e.g.[9]).

## 3. Coupled modeling approach of human and physics systems

To date, it is now possible to build a flexible coupled model wherein human agents are modeled by taking an MAS approach and implementing AI frameworks, in which the dynamics of physics systems (e.g., environmental systems like indoor spaces and building as well as urban physics systems)—governed by a set of transparent governing equations—are accounted for by a conventional simulation procedure (even though it is different from what von Neumann defined as a "simulation").

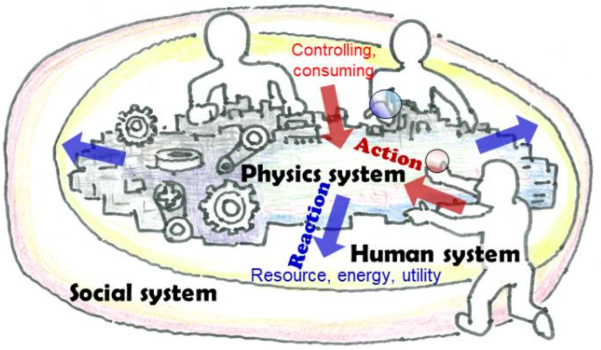
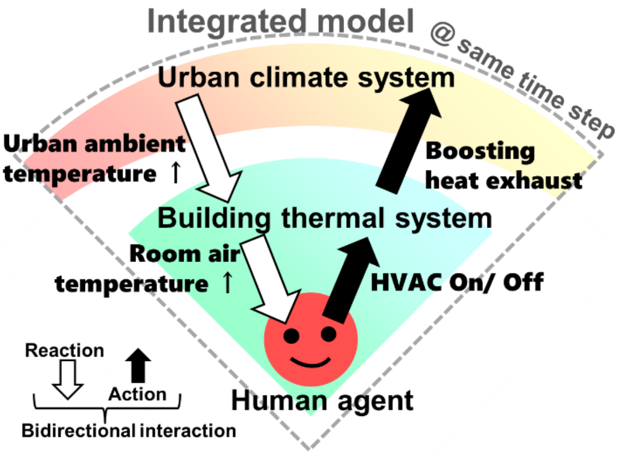



**Fig. 2:** Schematic explanation of how a physical system and a human system are mutually related through bilateral interactions. As can be seen, humans give actions (red arrows) to physical systems, such as natural environmental systems, to gain resources that are requisite for their survival. In return, the physical systems give reactions back to the human system (blue arrows). This feedback loop highlights the dynamics of both physical and human systems along spatiotemporal directions. Here, a complex behavior by each individual delivers the collective dynamics of the social system as a whole. We must keep the loop as sustainably healthy as possible because human beings cannot survive without relying on the resources we obtain from the surrounding physical systems.

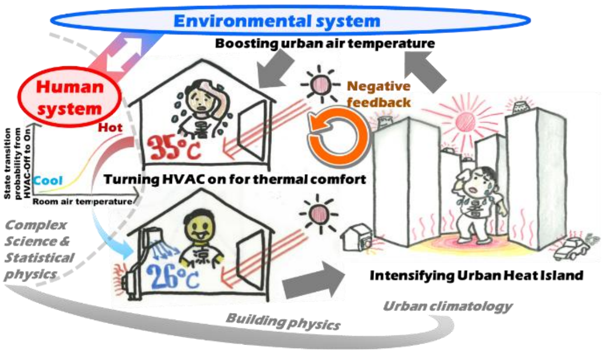
Let us consider why such a coupled framework connecting a human system with a physics system is so important. As shown in Fig. 2, any real system has complex interactions between the *human sphere* and the *physics system*, or more precisely, among the *human system*, *physics system*, and society, which is a collective entity of individuals whose dynamics sometimes differ from the simple superposition of "typical" individuals. The three systems are driven by three different principles and are mutually connected by the relations between action–reaction chains. When individuals (or say, society as a whole) try to extract much more benefit from a physics system (e.g., from the global environment) and if the agents take extreme action to it, the physics system may give back harsh reactions, which depend on the inherent potential of the physics system. For example, if each urban resident seeks individual utility optimization (e.g., maximizing individual thermal comfort), they will become overly reliant on HVAC (heating, ventilation and air-conditioning) systems backed by huge amounts of energy consumption during peak summer. This would inevitably lead to a more serious heat island phenomenon. Thus, we must see these three as an integrated system to accurately predict what happens and control it (if possible). To achieve this goal, we must develop a certain comprehensive model. This is the most important kernel of a human–physics system[10].

## 4. Human–physics system: integrated-type

A human–physics system requires a coupled model to connect two different domains: the physics and human system. In particular, if the human action (red arrow in Fig. 2) and reaction given back to the human (blue arrow in Fig. 2) are both significant, that is, if the bidirectional interaction is substantially heavy, the sub-model to quantify the dynamics of a physics system and another sub-model to demonstrate human action must be integrated, and these two parts should be treated as a fully simultaneous system from a mathematical point of view. We can call such a framework an *integrated model*.




(a)




(b)

**Fig. 3:** (a) Schematic of the concept of the proposed integrated model. All interactions are integrated simultaneously. Panel (b) illustrates the synergetic loop in a human–indoor space–building–urban environmental system[11,12].

At this point, I would like to cite an intelligible example, which refers to a framework used to analyze complex factors causing the urban heat island (UHI) phenomenon. A visual explanation of why the UHI phenomenon occurs is shown in Fig. 3. Panel (A) claims that in a physics system, a building thermal system is embedded in an urban climate system in a nested manner. The urban climate system is influenced by a resident's (human agent's) action of controlling HVAC systems to maintain their thermal comfort, which in turn drives up the urban air temperature through the increased exhausted heat emitted by the HVACs. Consequently, a positive feedback loop is established, which has a negative (unwilling) impact. The bidirectional action–reaction loop (depicted by black and white arrows in Panel (A)) cannot be ignored when modeling this complex system. Everything must be treated as simultaneous events. In comparison, Panel (B) shows this synergetic loop as more visually intelligible, which prompted us to build a human–indoor space–building–urban environmental comprehensive simulator, called AUSSSM, in 2004 (e.g.[11,12]).

## 5. Human−physics system: Cascade-type (CFD→MAS and MAS→CFD)

Again, highlighting the modeling approach for a human–physics system introduced in the previous section, we note that there is another type vis-à-vis the integrated-type, namely, the *cascade model*, where, unlike a bidirectional action–reaction loop, an interaction can be approximated by a one-way relation. In other words, the reaction can be negligible compared with the effect of an action. Let me introduce two examples, which are schematically visualized in Fig. 4.

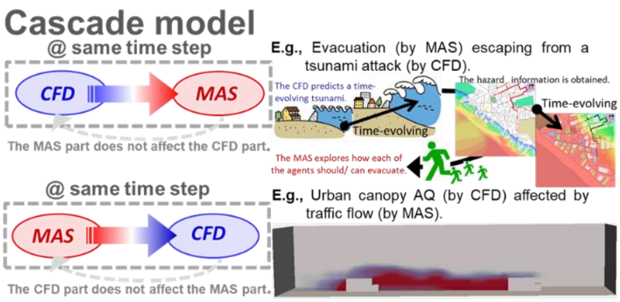



**Fig. 4:** Schema of the concept of the cascade model. As can be seen, twofold subordinates are possible if one intends to couple CFD and MAS. The upper panel illustrates a cascade model where the upward stage is modeled by MAS, while the downward stage is quantified by a CFD (denoted as the MAS→CFD model). In contrast, the bottom panel illustrates a cascade model where the CFD goes first, and subsequently, the MAS follows (denoted as the CFD→MAS model).

The first example is an evacuation simulation from a tsunami attack in a seashore area (upper panel), where a MAS to reproduce how each of the evacuees escapes the situation and a CFD to emulate the tsunami attack are implemented. The second example is a simulation of air quality in urban canopies (bottom panel), where a MAS to reproduce the dynamics of vehicles running and a CFD to reproduce the concentration of pollutants exhausted from the vehicles are coupled.

One might ask, "Why is only cascade treatment allowed and not integrated treatment?" In the first case, a tsunami (physics system) influences evacuees (human system), but evacuees do not influence the tsunami. Hence, the one-way cascade procedure is sufficient, in which the CFD applied to quantify the tsunami height goes first (upward part) in the entire simulation structure. This is then chased by an MAS (downward part) to allow evacuees to evade the tsunami attack based on each agent's temporal decision drawn from the individual information. These two stages occur at a same time step. Hereafter, we call this cascade the "CFD→MAS model." In the second case, the dynamics of vehicles, including acceleration, deacceleration, and lane-changes arouse the complex effect of turbulent mixing that determines the pollutant field represented by the concentration. Thus, the vehicles influence the concentration of pollutants, but the pollutants do not influence the vehicles' dynamics in general. Instead of exhausted gas from the vehicles, considering a lethal toxic gas diffusion (just as a hypothetical story), any driver's (vehicle) might be influenced. But, this is not the case we are now discussing. For this reason, an MAS to reproduce the vehicles' dynamics is used first, followed by a CFD to quantify the spatial distribution of pollutants. Let us call this cascade the MAS→CFD model.

Needless to say, a cascade-type model requires only lighter computational loads than an integrated-type model. This is because, in the case of an integrated model, all formulations must be treated simultaneously at a certain time step, irrespective of whether the physics or human system is involved. However, when considering a cascade model and comparing between the CFD→MAS and MAS→CFD models, the latter faces more serious difficulties than the former during actual computational processing. The key point is a huge gap in the time-discrete step size (e.g., $\Delta t$) between the CFD and MAS parts. The time scale of $\Delta t$ for a CFD is generally much less than that for a MAS, and such a gap may become $10^3$ order. Therefore, when a MAS goes first before a CFD, the MAS part's outputs from the two neighboring time steps (time-distancing $\Delta t_{\mathrm{MAS}}$ ) must be carefully interpolated to meet with $\Delta t_{\mathrm{CFD}}$. Otherwise, the MAS part cannot fairly provide the boundary condition to the CFD part. Meanwhile, in the CFD, moving vehicles are embedded in the CFD as still walls at each time step and for every $\Delta t_{\mathrm{CFD}}$. In contrast, in the case of CFD→MAS, such a problem does not matter because the CFD with a smaller time-discrete size than MAS ($\Delta t_{\mathrm{CFD}} \ll \Delta t_{\mathrm{MAS}}$) goes first, and this process requires none of the cumbersome interpolations required in other processes. This confirms that many evacuation simulators have been developed for tsunamis, floods, landslides, volcanic eruptions, building fires, and other practical situations considered as natural and artificial disasters.

Let us take a closer look at an MAS→CFD model to predict the spatiotemporal structure of HC (hydrocarbon) concentration, which originates from vehicles' exhausted gas. In particular, we want to determine how HC gas diffusion is intricately affected by the turbulent mixing effect brought about by running vehicles in the ditch of an urban canopy. Thus, the implementation to quantify the dynamics of each vehicle self-controlled by each driver depends on the driver's local circumstances. In particular, the current speed and headway gap to the preceding vehicle are requisite to the entire prediction framework, which is mainly composed of a MAS.

Figure 5 displays the results. For the MAS part, we adopted the Revised S-NFS model, one of the cellular automata models, which accounts for realistic car-following behaviors (including the so-called quick-start (QS), slow-to-start (S2S), and random braking (RB) effects, among others) and was validated by real traffic data (e.g.[11,13]). The model with assumption of $\Delta t_{\mathrm{MAS}}$=1 [s] predicts each vehicle's acceleration and speed at a certain time step, which in turn enables the prediction of HC gas exhaustion from each vehicle based on the VT-micro (Virginia Tech microscopic) model (e.g.[14]). Therefore, this upward simulation by the MAS provides the boundary conditions of (i) the vehicle's position and (ii) the production of HC gas for every $\Delta t_{\mathrm{MAS}}$.

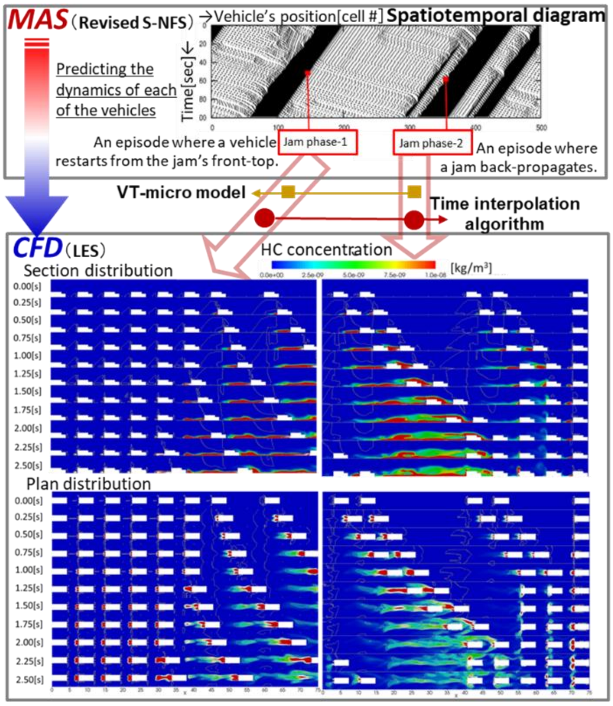



**Fig. 5:** An example of the MAS→CFD model. The model dovetails with the revised S-NFS model[11,13], reproducing the dynamics of human-driven vehicles with LES (e.g.[15]). This, in turn, reproduces the turbulent mixing of the exhausted gas from vehicles.

Meanwhile, we adopted a large eddy simulation (LES) for the CFD part, which follows the MAS part. Our LES (e.g.[15]) with a presumption of $\Delta t_{\mathrm{CFD}}=10^{-3}$ [s] can predict the unsteady distribution of HC concentrations based on the boundary condition delivered by the MAS part. As mentioned above, to bridge the gap of $\Delta t_{\mathrm{MAS}}$ and $\Delta t_{\mathrm{CFD}}$, we developed an efficient and smooth time interpolation algorithm. However, the computational load is so heavy that it drives us to focus on a very limited space out of the entire domain. As shown in the spatiotemporal diagram (where each dot shows the position of a vehicle at a moment) as the inset in Fig. 5, we pick up two episodes. One is a scenario where a head vehicle in jam restarts, thus moving away from the jam cluster (Jam phase-1). Another is a scenario where vehicles approach the tail of a jam cluster one by one (Jam phase-2). The bottom panels display the respective snapshots of the two episodes. Here, we can clearly understand how turbulent mixing brought about by the dynamics of vehicles can be visually captured (see movies in the supplementary materials).

## 6. Concluding remarks

CFD has become a common tool used to quantitatively predict any flow field: indoor air, urban air, seawater, pipe flow water, even tsunamis, and whatever we intend to deal with as long as it is fluid. Nowadays, we can rely on various software, whether it is open and free or commercialized (paid basis). CFD enables us to predict the complex dynamics of air temperature, wind speed, gas concentration, water flow rate, tsunami wave height, and the information of higher stochastic moments of those physical properties, such as kinetic energy, brought about by the turbulent effect of a fluid flow. Such a sophisticated prediction is delivered by a well-devised numerical solution for a set of governing equations, namely, the 3D Navier–Stokes equations.

Meanwhile, MAS, in this context, quantifies the dynamics of complex human action. Each agent (i.e., particles) represents each individual in a model. MAS predicts the moving dynamics of each pedestrian, evacuator, vehicle (driver), and various other human (driven) agents. In the case of an evacuation simulation, an MAS predicts how each evacuator moves (i.e., to which direction and how fast an agent walks or runs). Each agent's decision-making process depends on the local environment, thereby implying the local information that can be obtained by the focal agent, the surrounding situation about neighboring evacuees, and additional information given to them by emergency broadcast through radio and IoT devices, for example.

Needless to say, the frameworks of CFD (applied to the physics system) and MAS (applied to the human system) are given as different simulation bodies, and each might be given as a complete program. Then, we come to a specific question: whether it would be integrated or cascade, whether it is placed in an upward position in the entire simulation flow, and whether it is MAS or CFD when a cascade-type model is allowed. The present article provides some concrete examples concerning the cascade-type coupling model, thereby highlighting the fact that the MAS→CFD model is more difficult than the CFD→MAS model.

Meanwhile, what can we see and should capture in the sphere of 'simulation' for the scientifically valuable picture? It might be the most important and heavily concerned question to the readers of Journal of Building Performances and Simulations, which is one of the general questions in building physics. As the present report shows, the organic alliance of CFD with MAS is extremely powerful in elucidating many complex phenomena where a building physics system and the human entity have mutual-permeating relations. Although there might be some technical problems such that a CFD requires a finer time resolution than a MAS does, I am personally optimistic because pursuing many engineering applications urges us to solve the impediment.

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## Supplementary materials

The hyperlinks show the animation clips of what Figure 5 explains above, where (i) the Free-flow phase, (ii) Jam phase-1, and (iii) Jam phase-2 are delivered.

## References

1) Ulam, S., Richtmyer, R. D., von Neumann, J.; Statistical methods in neutron diffusion, *Los Alamos Scientific Laboratory Report* LAMS–551, (1947). doi.org/10.1525/9780520322929-004.
2) Tanimoto, J., Hagishima, A., Tanaka, Y.; Study of bottleneck effect at an emergency evacuation exit using cellular automata model, mean field approximation analysis, and game theory, *Physica A* 389 (24), 5611-5618, (2010). doi.org/10.1016/j.physa.2010.08.032.
3) Hossain, M. A., Kabir, K. M. A., Tanimoto, J.; Improved car-following model considering modified backward optimal velocity and velocity difference with backward-looking effect, *J. Appl. Math. Phys.* 09 (2), 242-259, (2021). doi.org/10.4236/jamp.2021.92018.
4) Karplus, W. J.; The spectrum of mathematical modeling and systems simulation, *Math. Comput. Simul.* 19 (1), 3-10, (1977). doi.org/10.1016/0378-4754(77)90034-9.
5) Rosenblatt, F.; The perceptron: A probabilistic model for information storage and organization in the brain, *Psychol. Rev.* 65 (6), 386-408, (1958). doi.org/10.1037/h0042519.
6) Anthony, M., Neural Network; Learning: Theoretical

Foundations, Cambridge University Press, 2009.

7) Sutton, R. S., Barto, A. G.; Reinforcement Learning ($2^{nd}$ edition), Bradford Publishing, 2018.
8) Goodfellow, I., Bengio, Y., Courville, A., Learning, D., MIT Press, 2016.
9) Sharma, G., Guo, H., Shen, C., Tanimoto, J.; Small bots, big impact: Solving the conundrum of cooperation in optional prisoner's Dilemma game through simple strategies, J. R. Soc. Interface 20 (204), 20230301, (2023). doi.org/10.1098/rsif.2023.0301.
10) Tanimoto, J.; Sociophysics Approach to Epidemics, Springer, 2021.
11) Tanimoto, J.; Evolutionary Games with Sociophysics: Analysis of Traffic Flow and Epidemics, Springer, 2019.
12) Tanimoto, J., Hagishima, A., Chimklai, P.; An approach for coupled simulation of building thermal effects and urban climatology, *Energy Build.* 36 (8), 781-793, (2004). doi.org/10.1016/j.enbuild.2004.01.019.
13) Kokubo, S., Tanimoto, J., Hagishima, A.; A new cellular automata model including a decelerating damping effect to reproduce Kerner's three-phase theory, *Phyisica A* 390 (4), 561-568, (2011). doi.org/10.1016/j.physa.2010.10.027.
14) Rakha, H., Ahn, K., Trani, A.; Development of VT-Micro model for estimating hot stabilized light duty vehicle and truck emissions, *Transp. Res. D Transp. Environ.* 9 (1), 49-74, (2004). doi.org/10.1016/S1361-9209(03)00054-3.
15) Abd Razak, A. A., Hagishima, A., Ikegaya, N., Tanimoto, J.; Analysis of airflow over building arrays for assessment of urban wind environment, *Building and Environment* 59, 56-65, (2013). doi.org/10.1016/j.buildenv.2012.08.007.