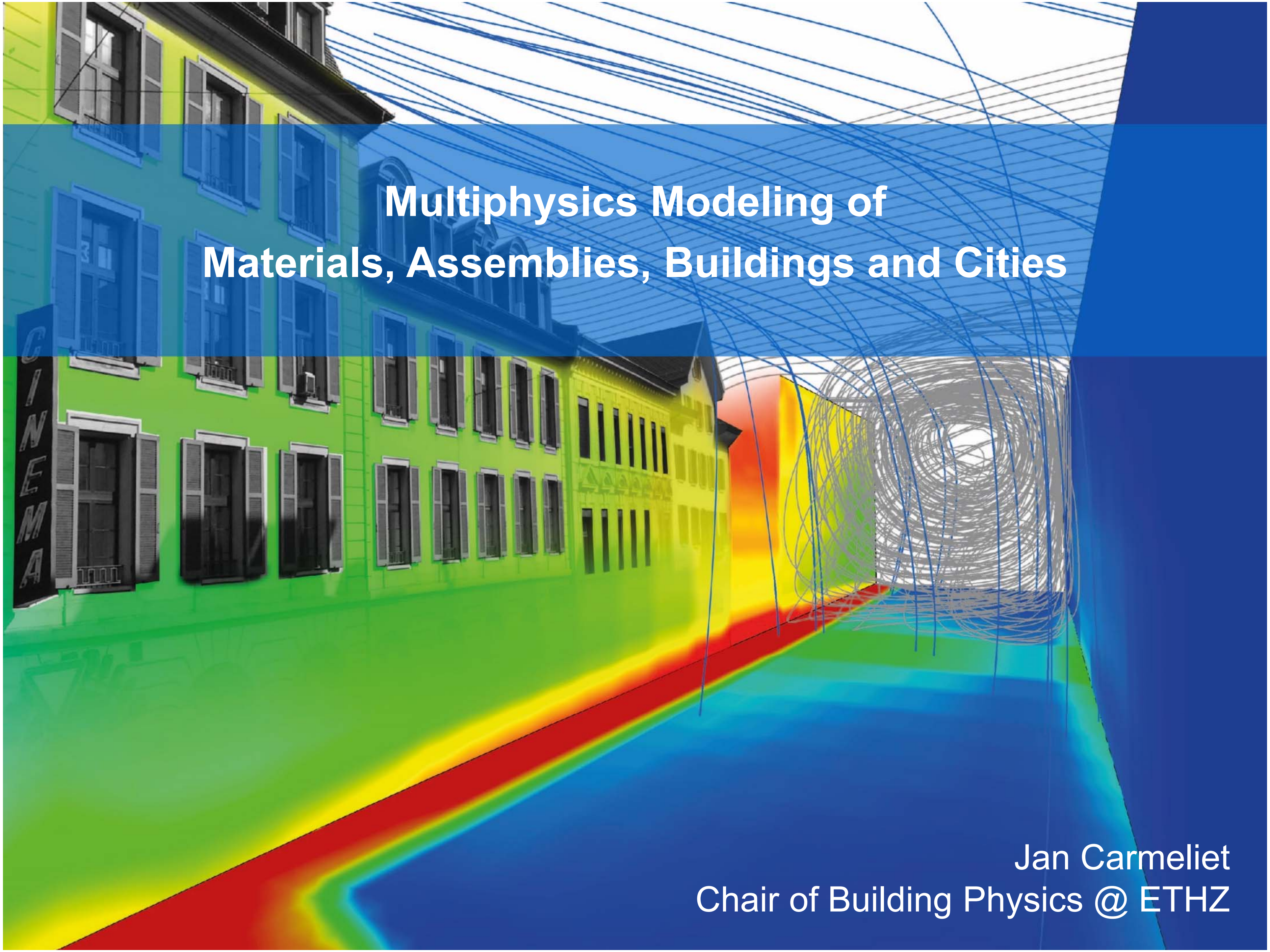
Multiphysics Modeling of Materials, Assemblies, Buildings and Cities



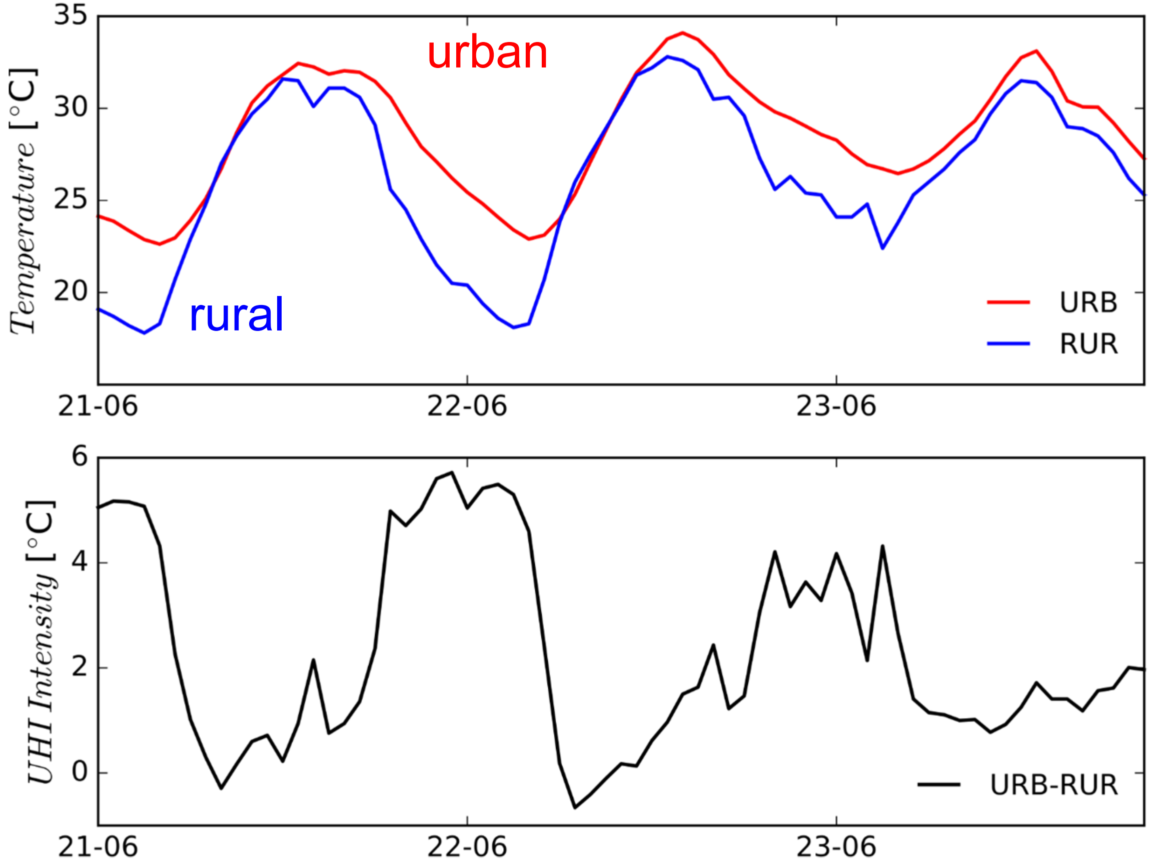
Jan Carmeliet
Chair of Building Physics @ ETHZ

Urban climate for Zürich, Switzerland

Touristic info: Climate with no excessive heat, cold nor humidity

Zurich experienced heat wave June 2017

Air temperature at 2 m

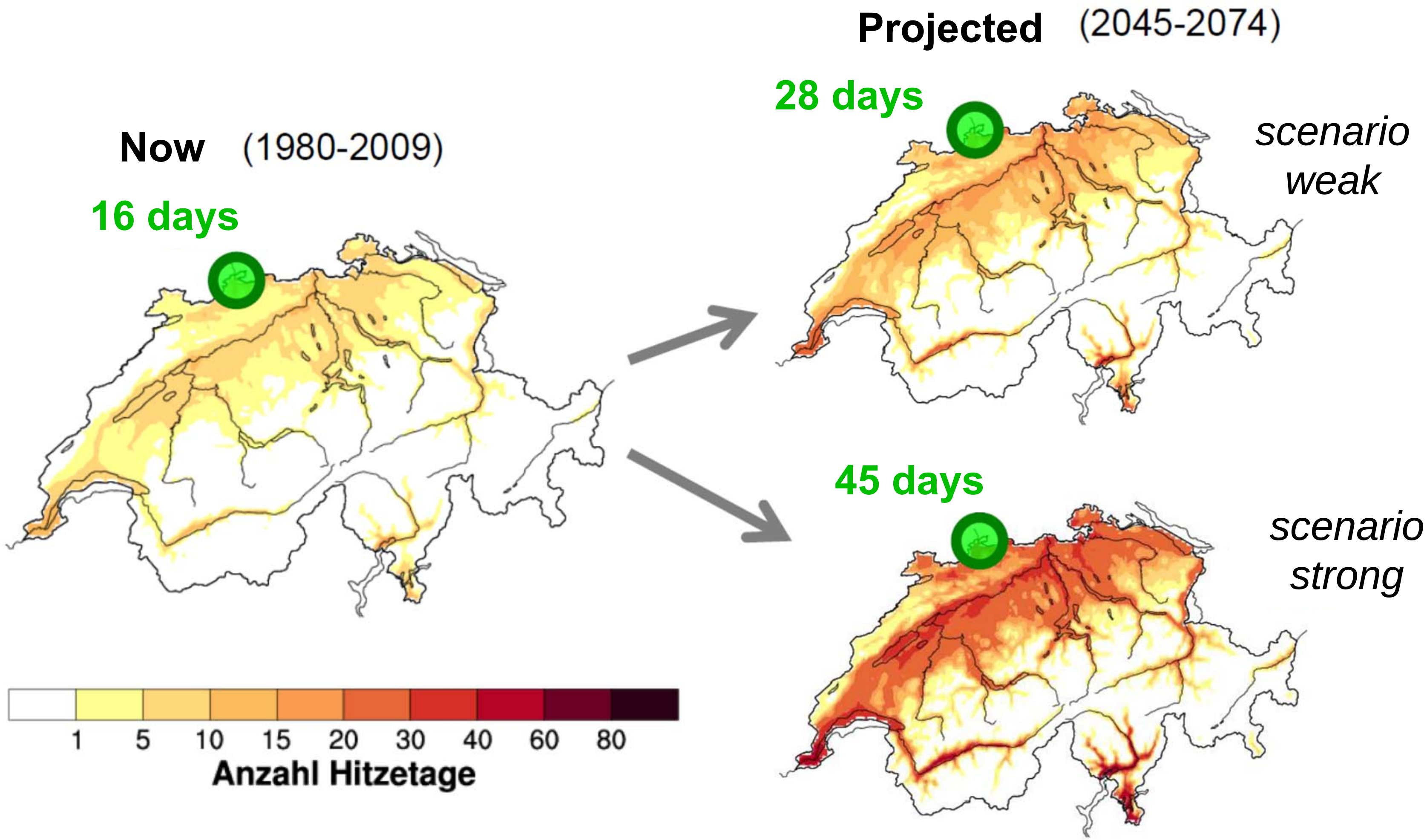


Urban heat island intensity

*Urban air temperature – rural air temperatur*e

higher daytime temperatures, reduced night-time cooling

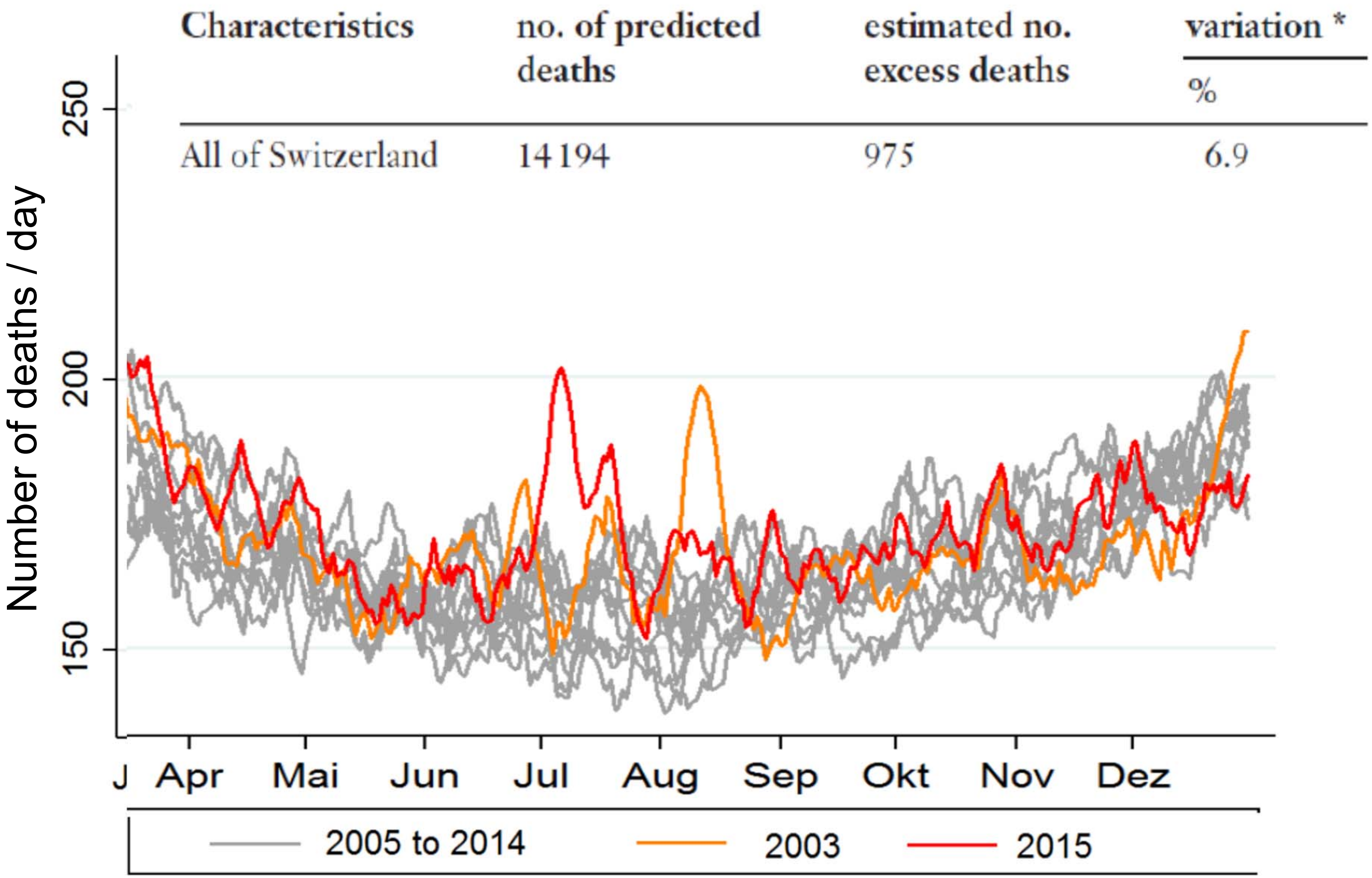
Climate change and heat days (T≥30°)



infras DENKEN ÜBER MORGEN

(Infras/BAFU 2014, Zubler et al. 2014)

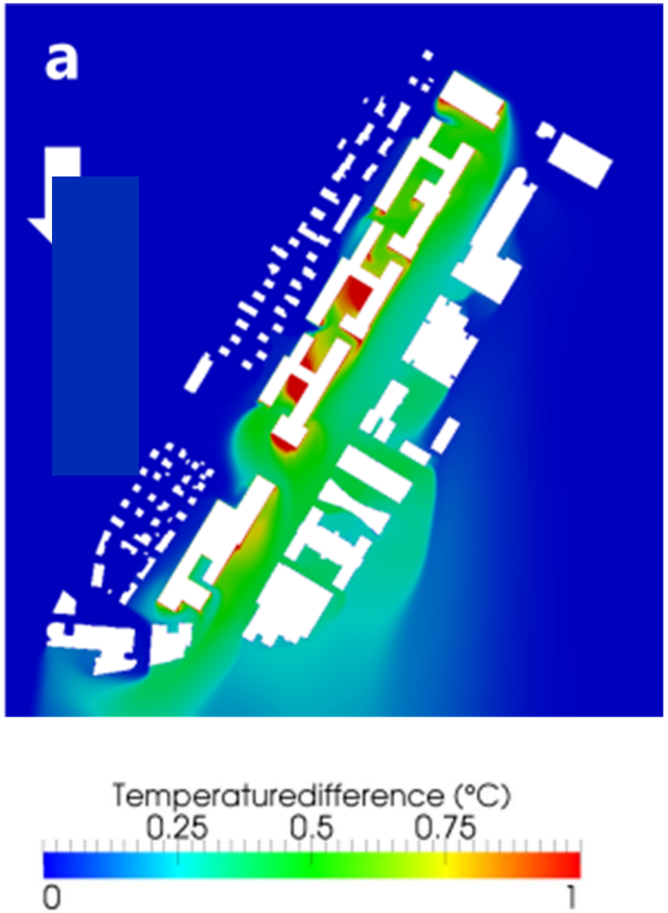
Excess mortality
during the heat waves of summer 2003 and 2015



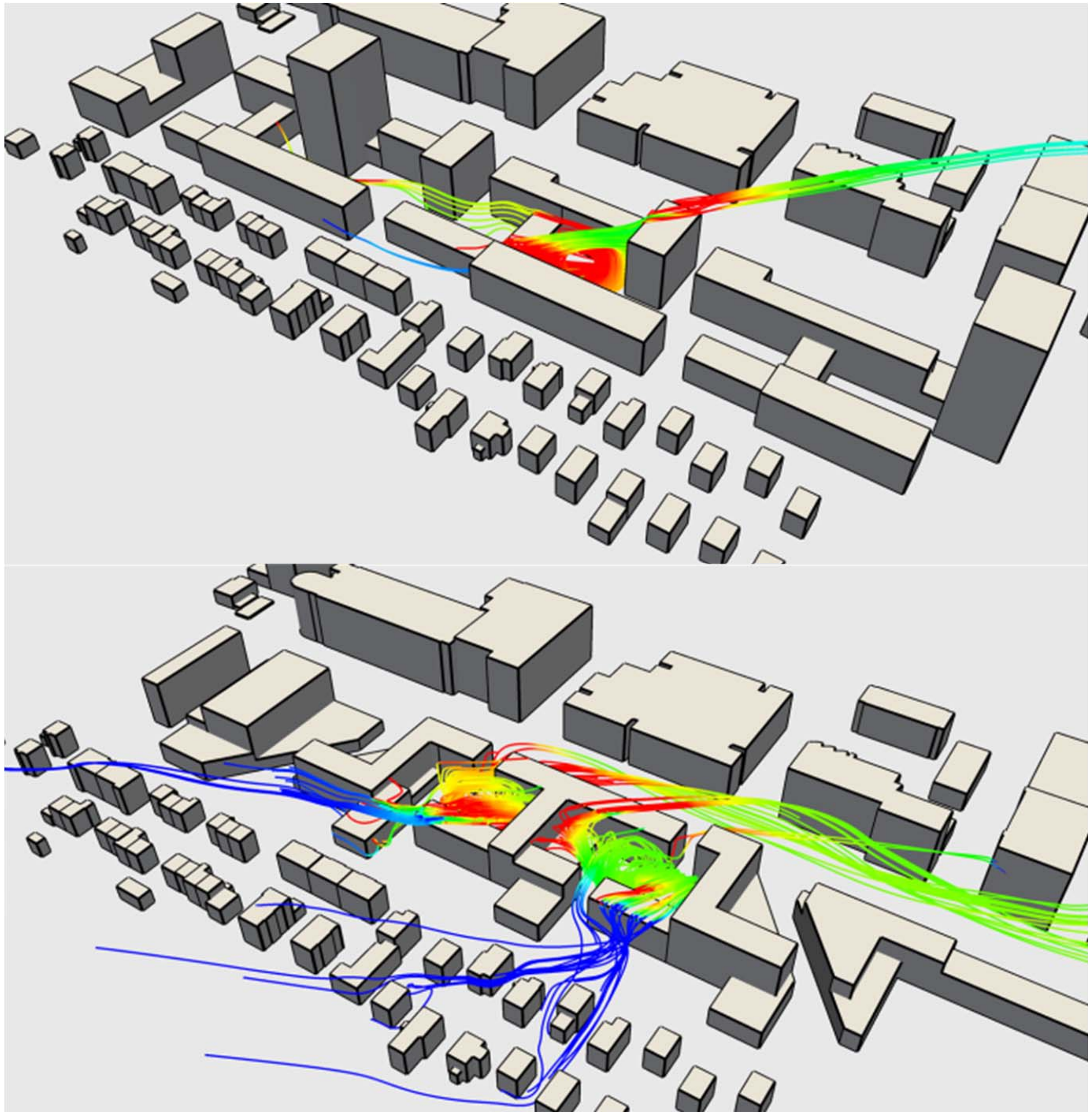
(SwissTPH, 2016)

Local heat island (hot spots) appears at street canyon scale

Case study of densification in Zurich

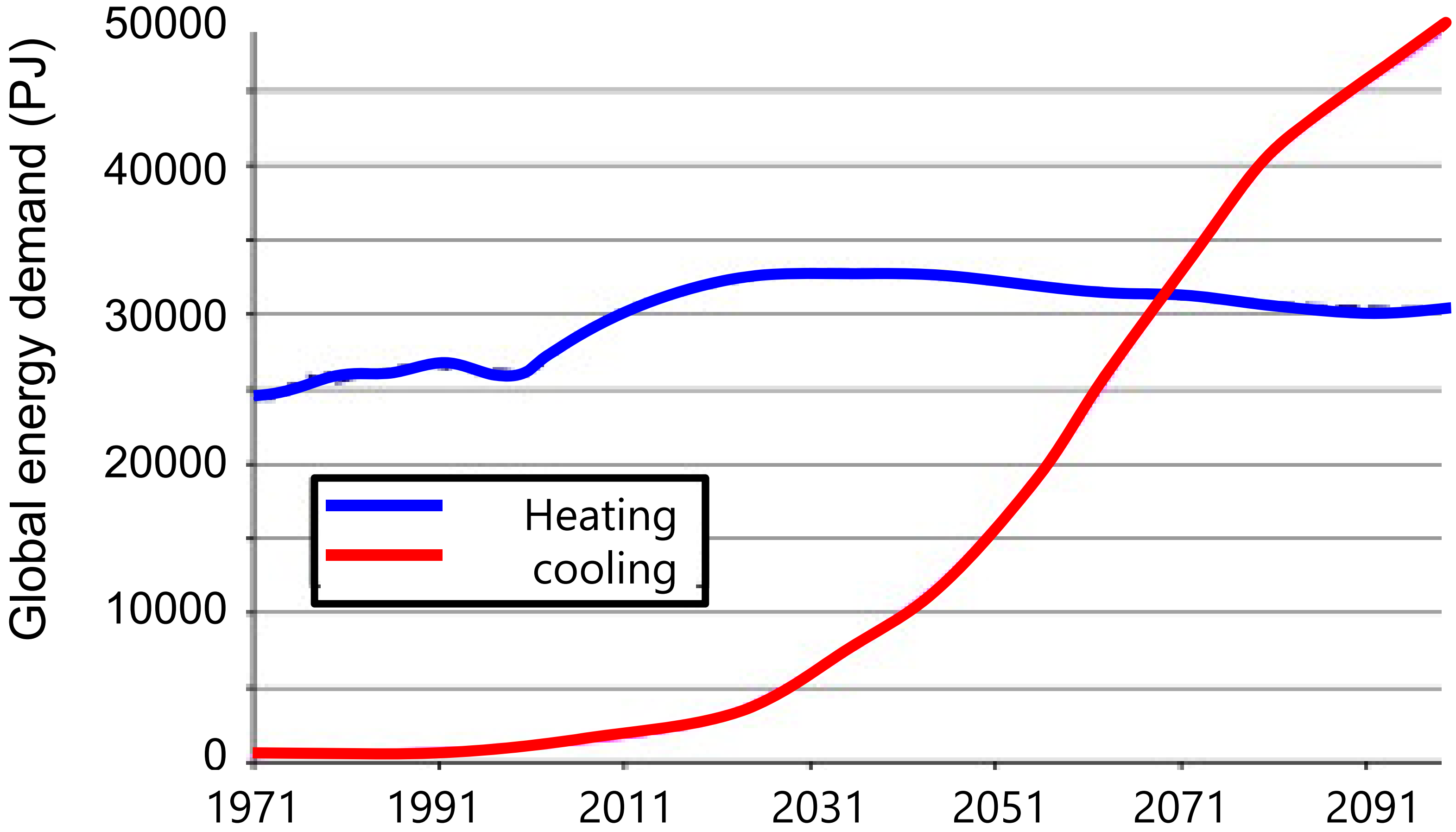


temperature difference between the local and ambient air temperature



Global residential energy demand with climate change

reference scenario



Increase cooling demand from 4.4 % to 35 % in 2050 and 61% in 2100

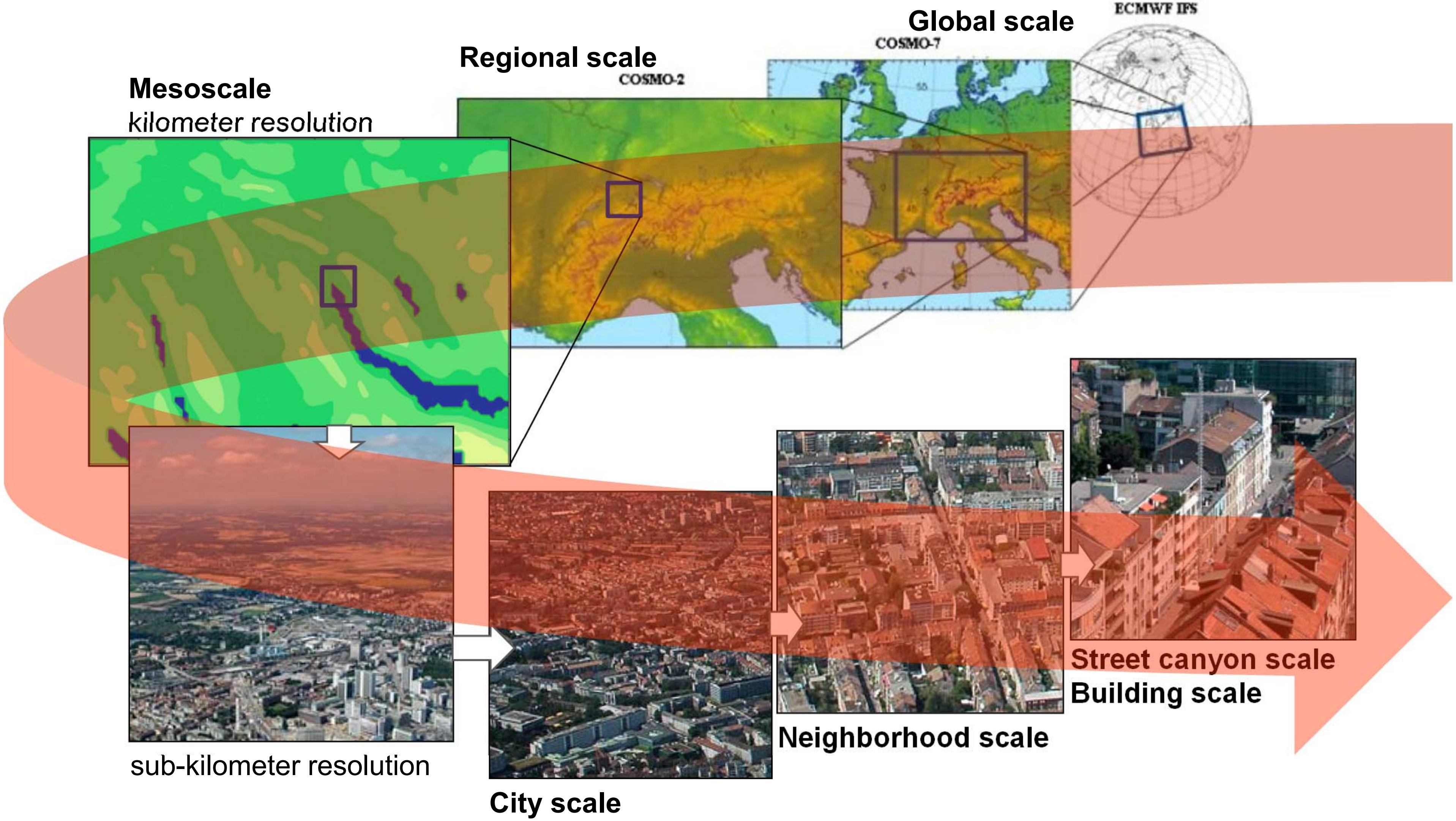
Isaac and van Vuuren 2009

Observations

- Climate change: heat waves are becoming more frequent under increasing greenhouse forcing
- Urban heat island (UHI) effect is growing
- Appearance of local heat islands

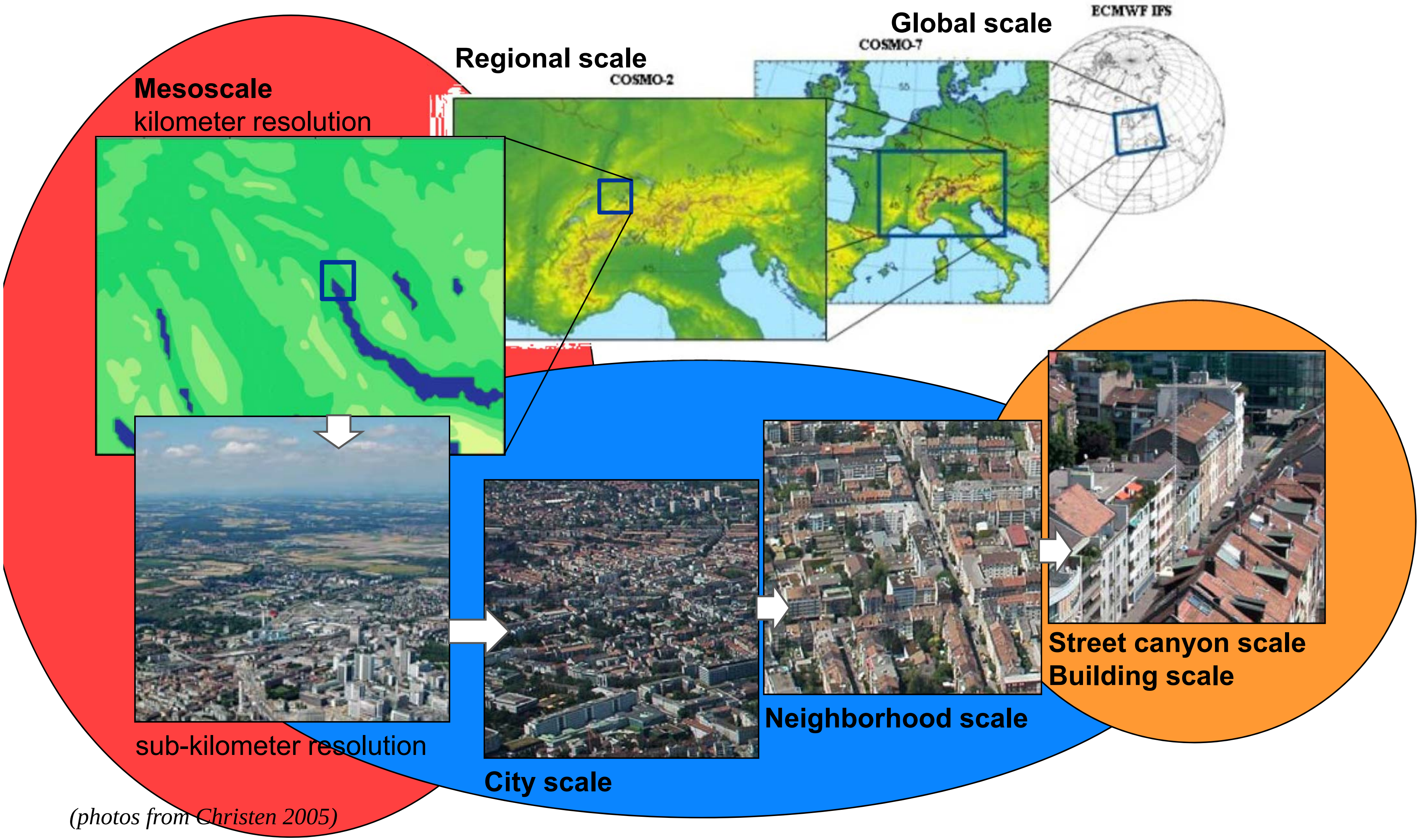
SCALES in Urban climate

downscaling



(photos from Christen 2005)

SCALES in Urban climate



(photos from Christen 2005)

Observations

- Climate change: heat waves are becoming more frequent under increasing greenhouse forcing
- Urban heat island (UHI) effect is growing
- Appearance of local heat islands
- **Urban climate is multiscale problem**

Questions

What is impact of urban and local climate under climatic change on

- Urban thermal comfort, heat stress, health (pollutants)
- Building & urban (cooling) energy demand
- Hygrothermal performance and durability of building envelopes

Questions

What is impact of urban and local climate under climatic change on

- Urban thermal comfort, heat stress, health (pollutants)
- Building & urban (cooling) energy demand
- Hygrothermal performance and durability of building envelopes
- ….
- Link to indoor air quality, indoor comfort
- Link to urban water management, flooding, ….

Challenges

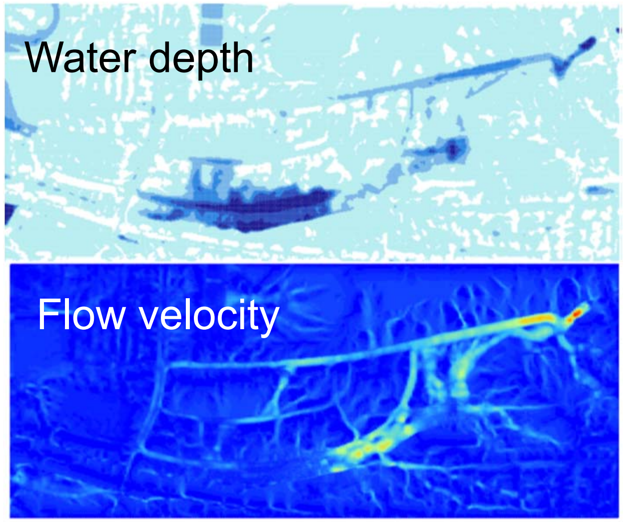
Develop urban heat island mitigation strategies on different scales:

1. Regional and urban scale

- Adequate regional adaptation measures for climate change (CC) decreasing greenhouse gas forcing
- Clever regional land use and urban radiation management (higher albedo)
- Clever use of water resources: storm water storage, grey water

Land (unploughed), brighter crop species, white infrastructure (cities)

Sonia I. Seneviratne et al 2018



Surface run-off model on urban scale

J.P. Leitao et al. 2016

Challenges

Develop urban heat island mitigation strategies on different scales:

1. Larger regional and urban scale
2. Local urban scales (street canyon, buildings)

- Adequate global and local urban heat island mitigation measures
- Cool surfaces (albedo, evaporative cooling), shadowing, urban ventilation, vegetation

New breakthrough necessary

Urban physics

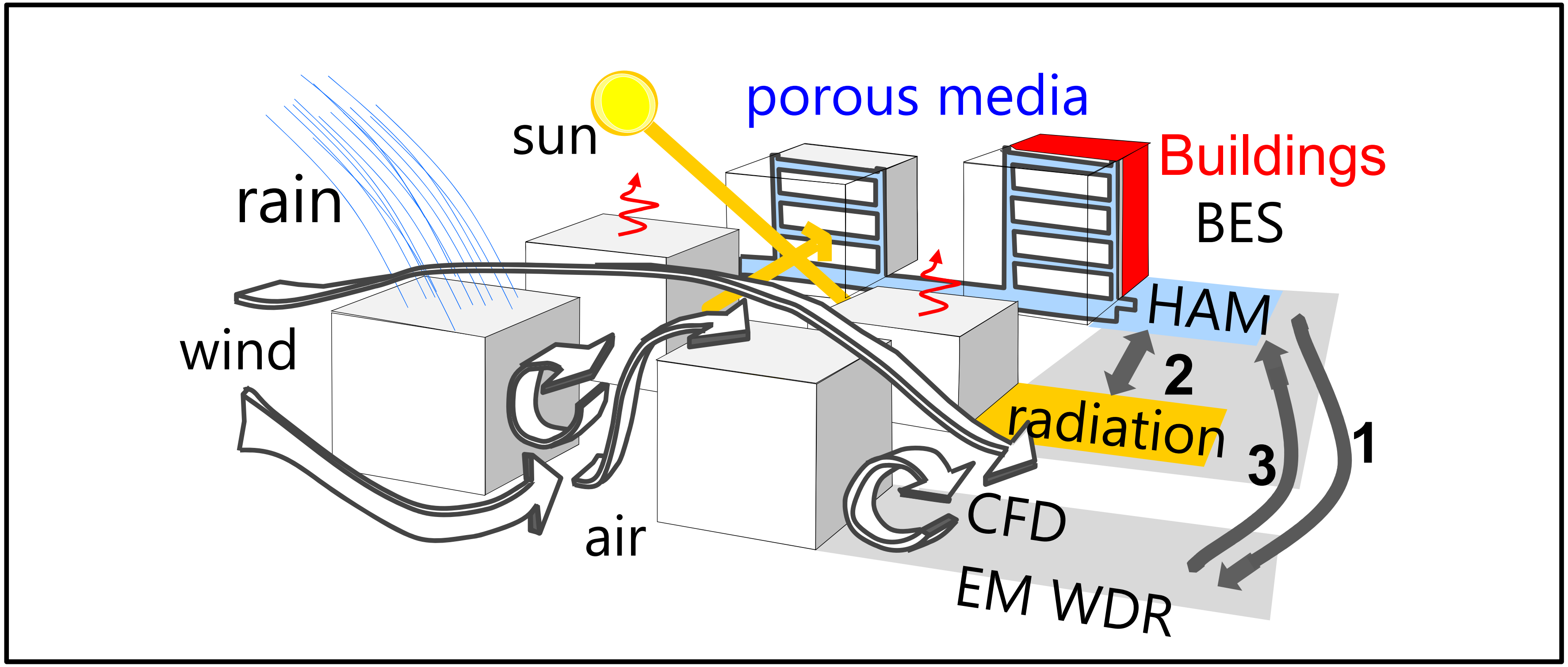
Building physics

Unified approach

All-physics approach

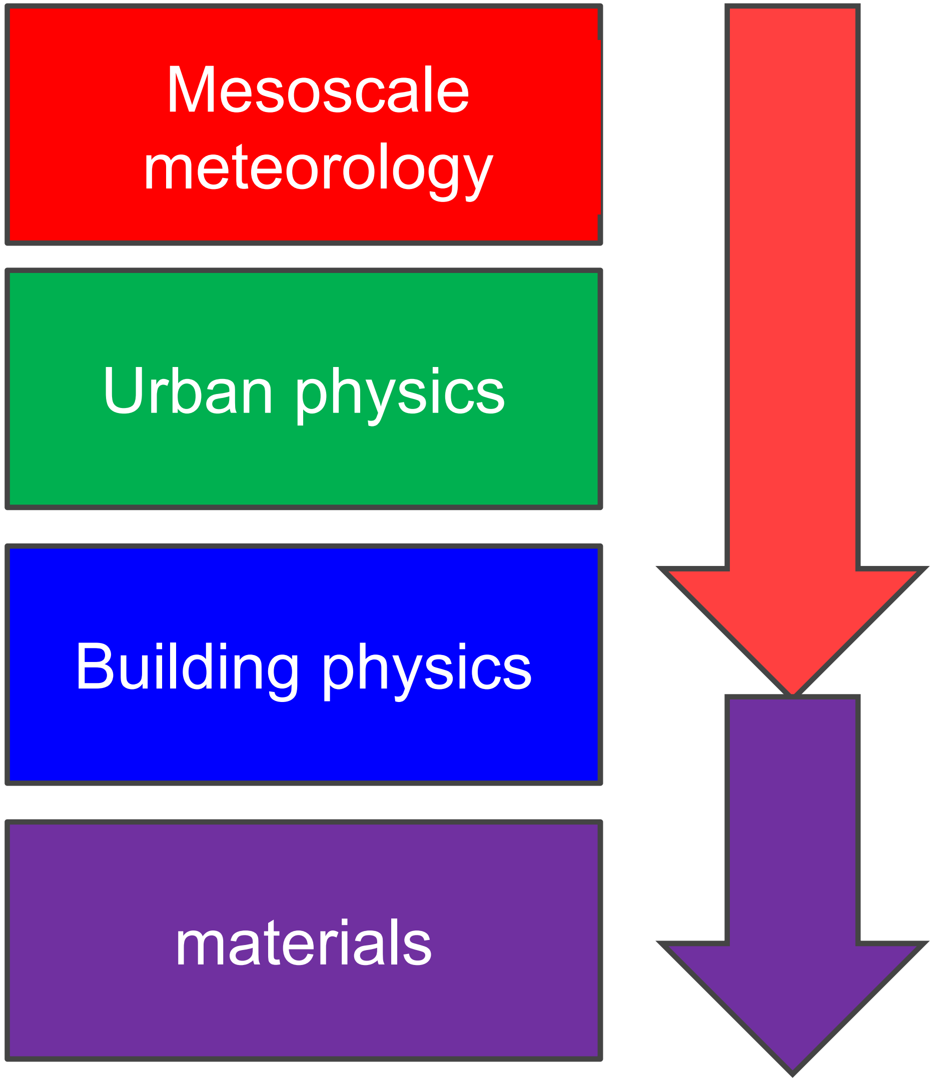
- experiments and modelling
- Over scales of materials to buildings and cities

All physics coupled model for urban climate and buildings



HAM	heat and moisture transport in porous materials (building materials, pavements, soils, …) including phase change: evaporative cooling
CFD	air flow due to wind and buoyancy
WDR	wind driven rain, Eulerain multi-phase model
Radiation	short and longwave radiation using view-factor method
BES	building enery simulation

New breakthrough necessary

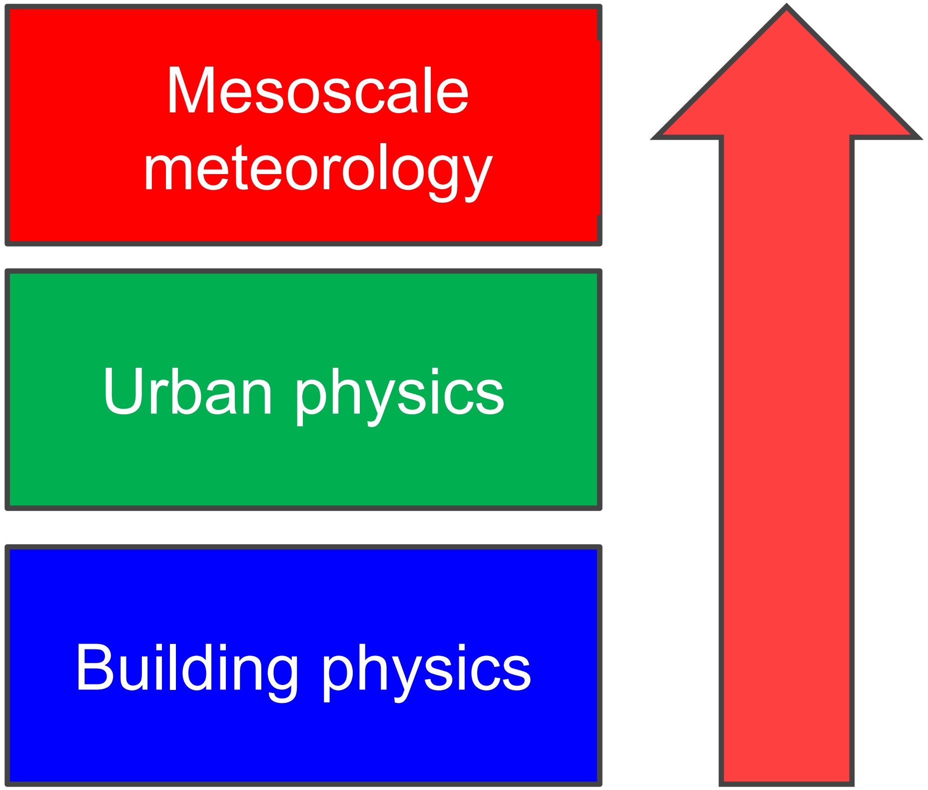


Coupled approach

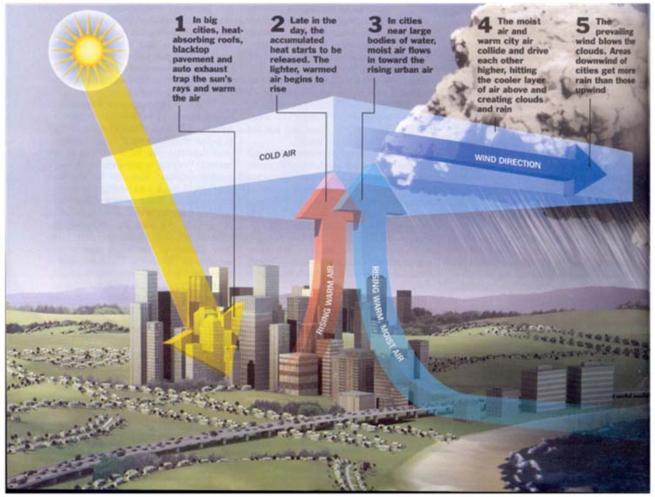
Downscaling
from **regional mesoscale meteorological** models

towards urban, building
and **material scales**

New breakthrough necessary

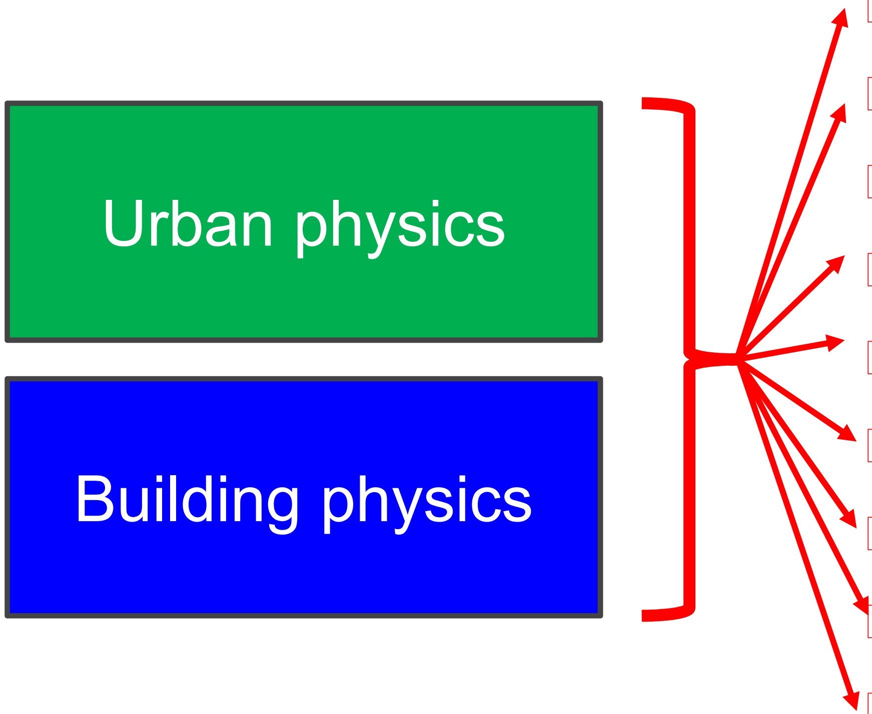


Upscaling: impact of city on regional climate



From TIMES magazine, Aug 2003

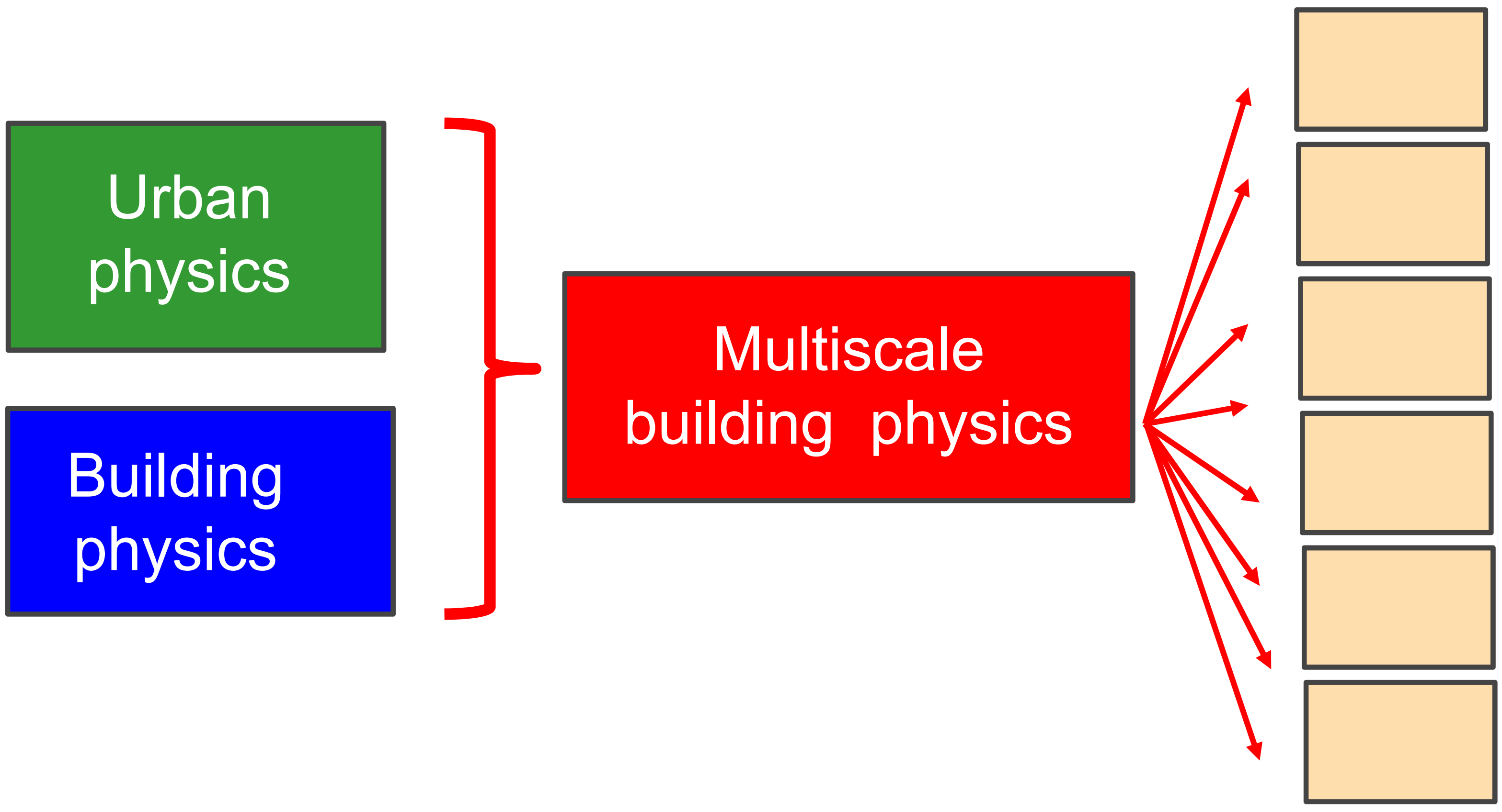
New breakthrough necessary



Interdisciplinary approach

- atmospheric and climate science
- urban meteorology
- urban water management
- health sciences
- thermal physiology and comfort
- material science
- urban design
- …….
- …….

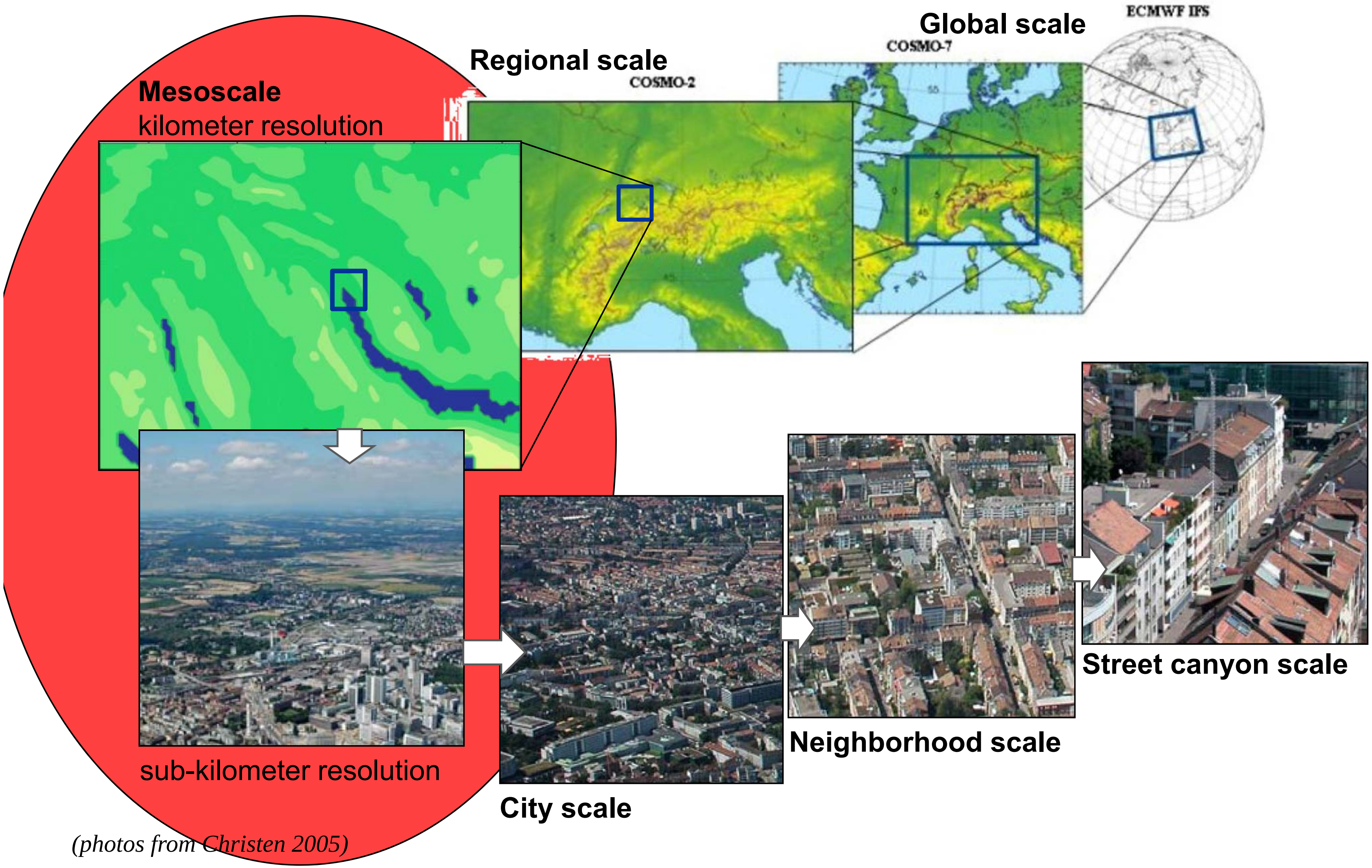
New breakthrough necessary



New breakthrough necessary

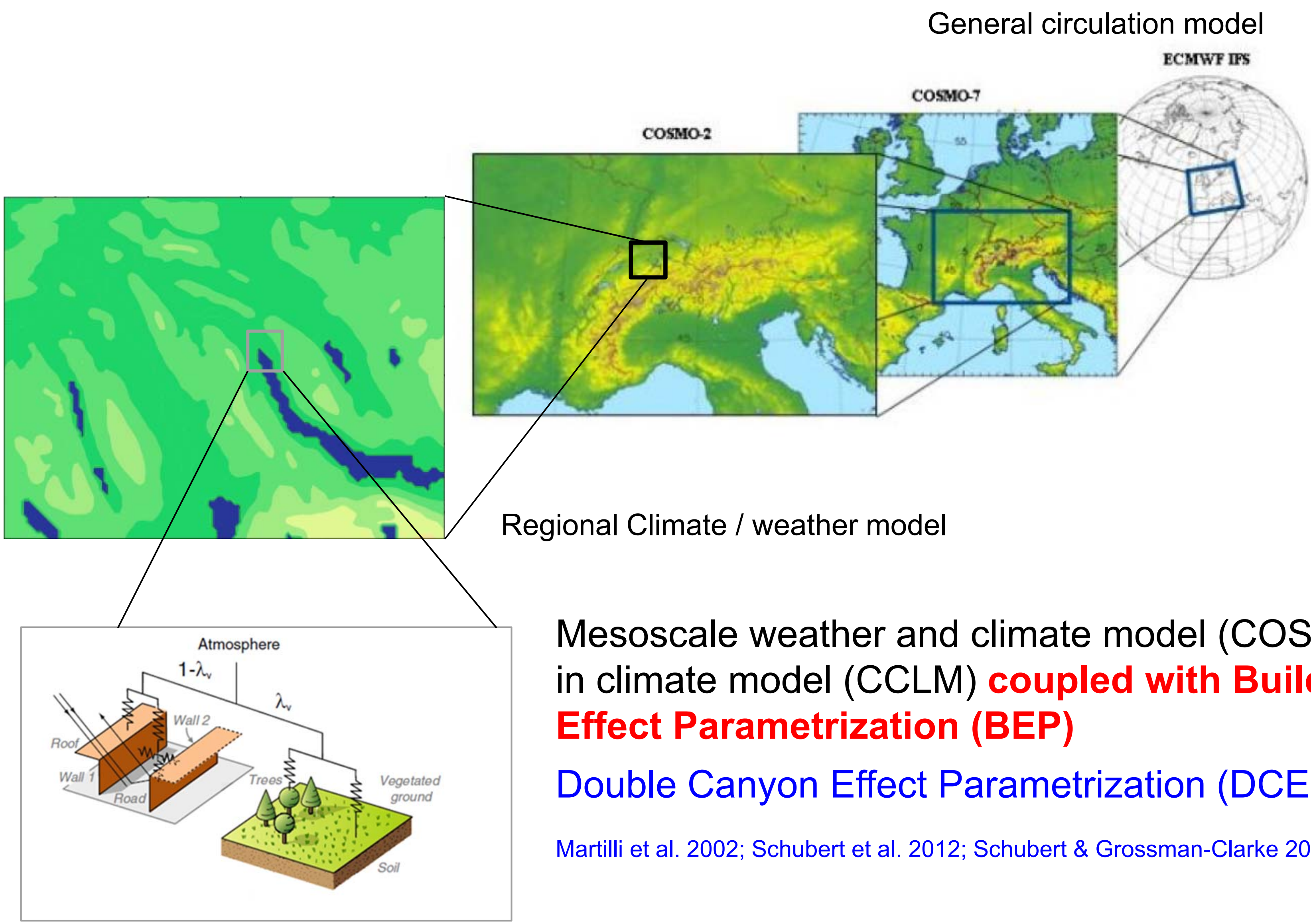
Multiscale building physics

SCALE 1: mesoscale



(photos from Christen 2005)

Mesoscale Meteorological Model & Urban Parametrization



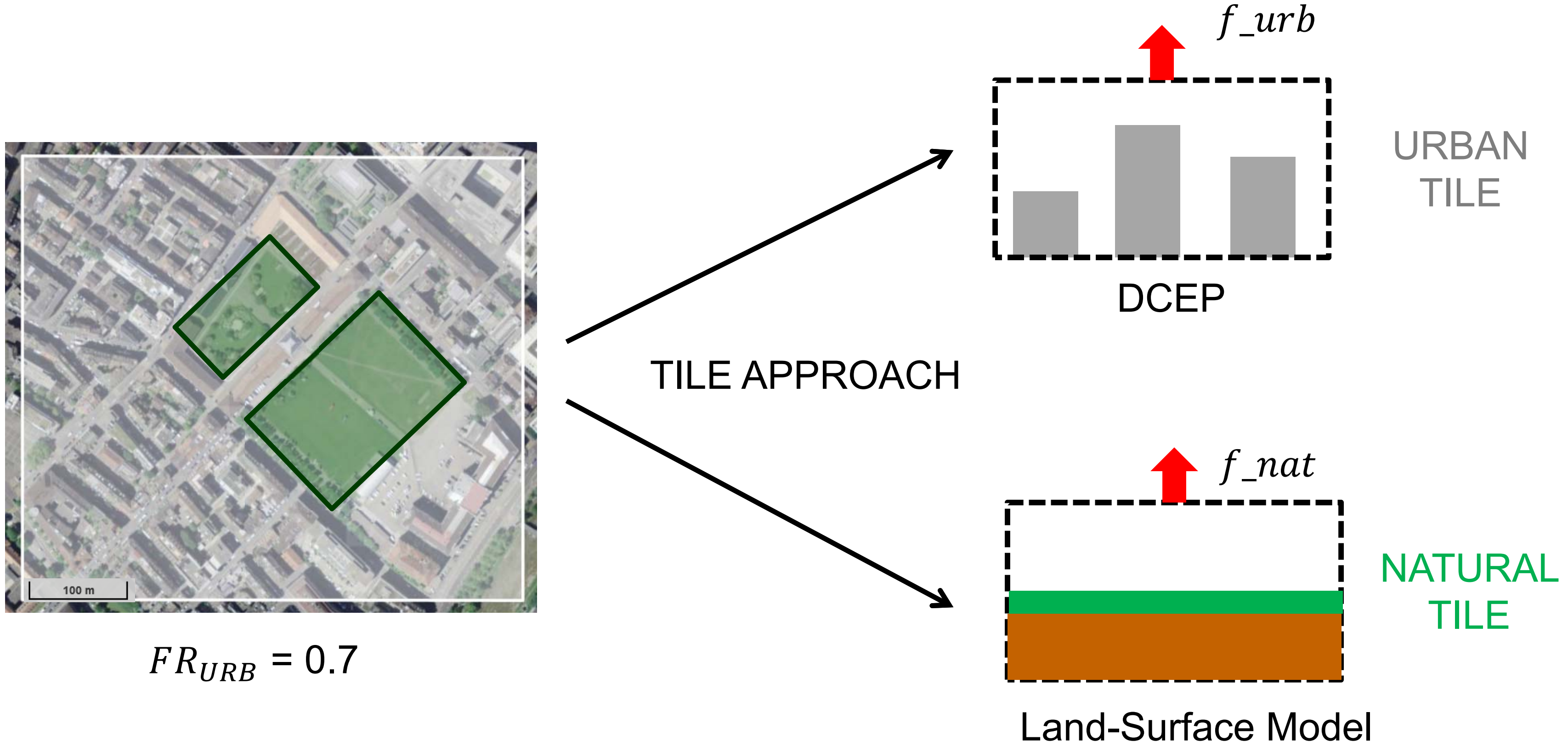
Mesoscale weather and climate model (COSMO) in climate model (CCLM) **coupled with Building Effect Parametrization (BEP)**

Double Canyon Effect Parametrization (DCEP)

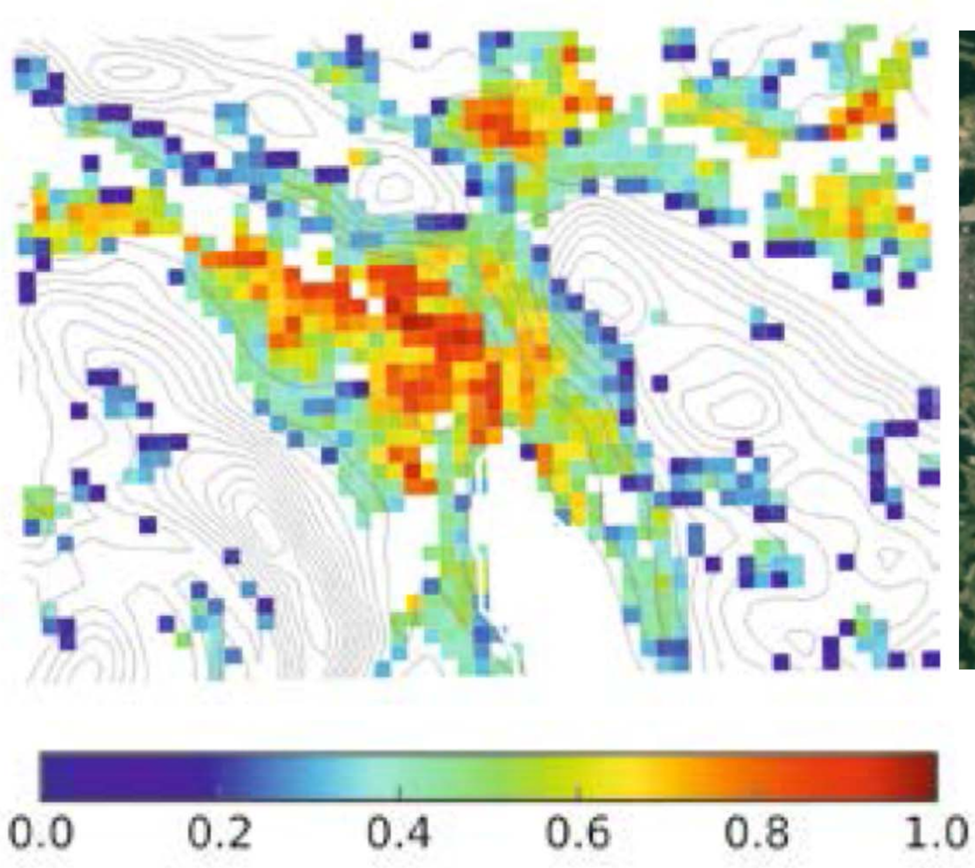
Martilli et al. 2002; Schubert et al. 2012; Schubert & Grossman-Clarke 2014

Parametric model : DCEP urban canopy model

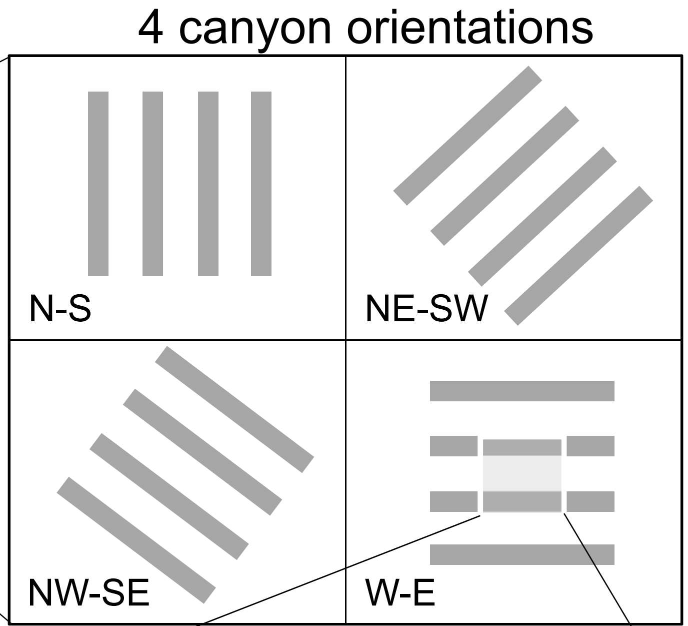
Tile approach: urban and natural fraction



Urban fraction for Zurich

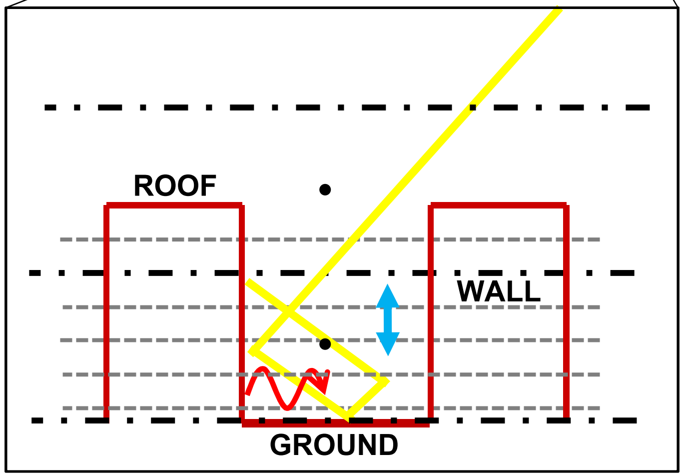


Parametric model : urban canopy model



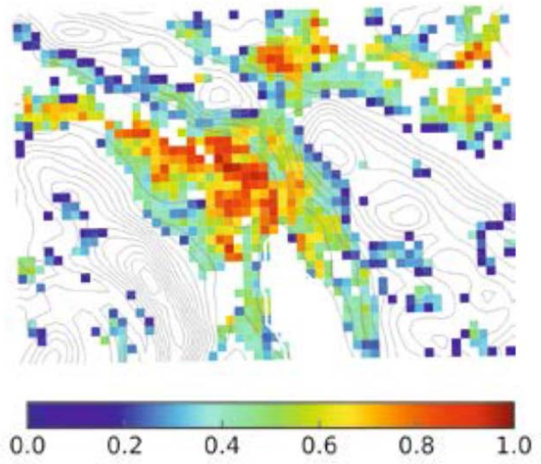
Double Canyon Effect Parameterization (DCEP)

- multi-layer model
- 3 active surfaces
  - Roofs
  - Wall
  - ground

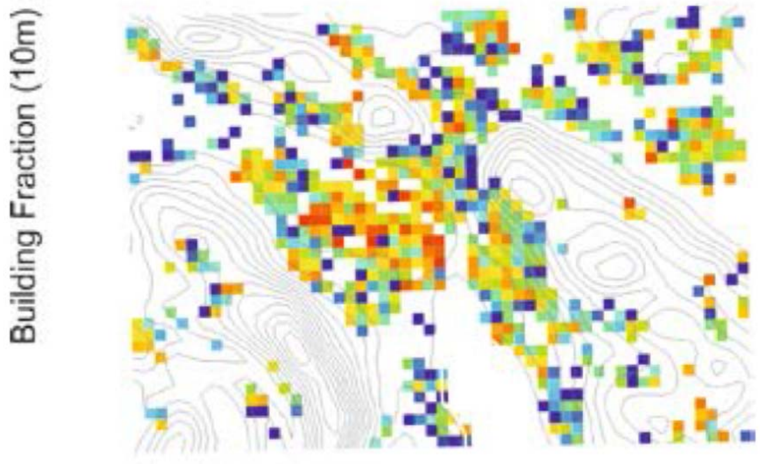


Urban fraction and building fraction

Urban fraction

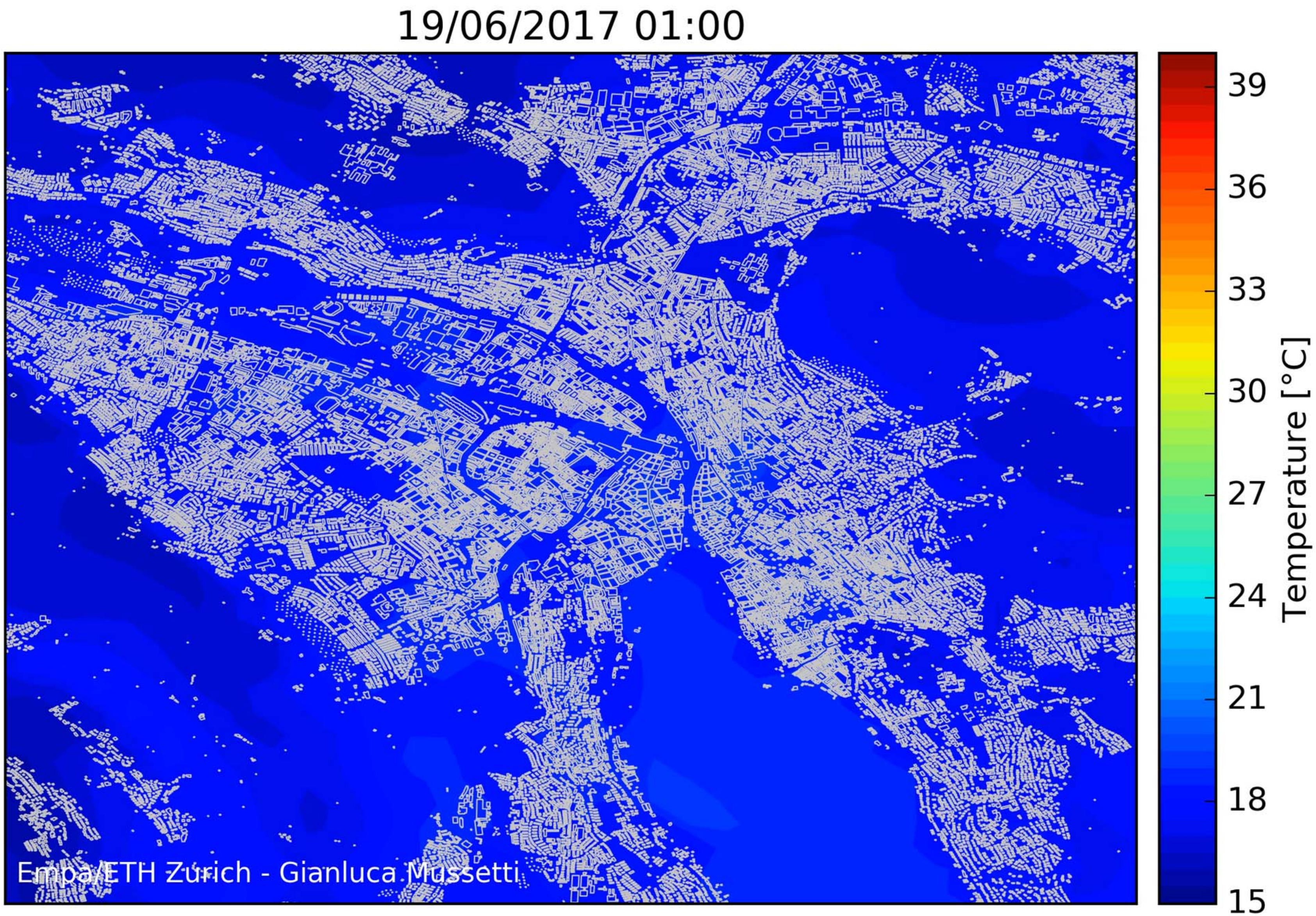


Building fraction (10m)



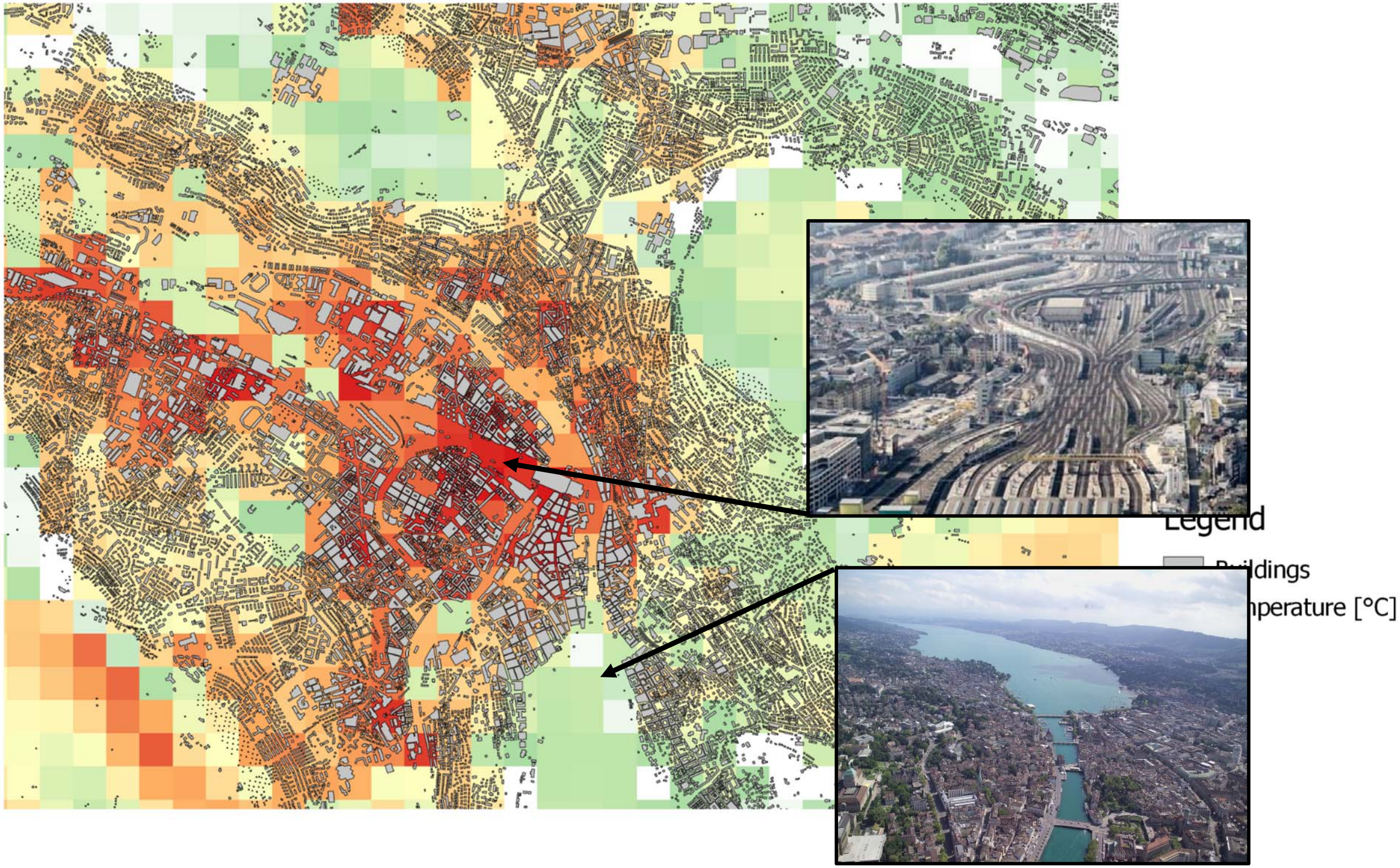
	Roofs	Walls	Streets
Albedo	0.15	0.1	0.1
Emissivity	0.9	0.9	0.95
Heat capacity [$J\ m^{-3}\ K^{-1}$]	2.3×10^{6}	2.3×10^{6}	2.3×10^{6}
Thermal diffusivity [$m^{2}\ s^{-1}$]	0.67×10^{-6}	0.67×10^{-6}	0.29×10^{-6}

Zurich experienced heat wave June 2017



Zurich experienced heat wave June 2017

Air temperature map at 6 am 23/06/2017



Why the air temperatures in cities are so high during a heat wave?

Heat storage during heat wave

Storage flux =

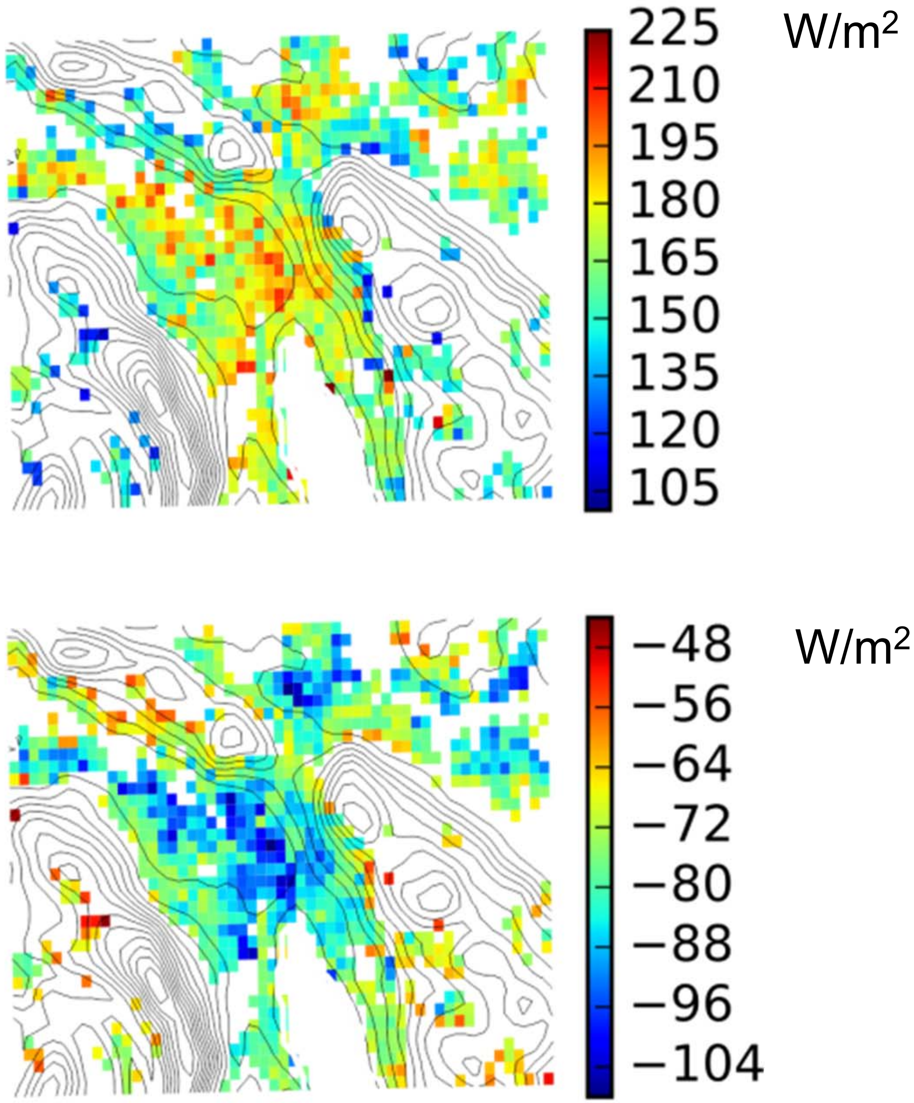
net radiation income – sensible heat – latent heat

Heat storage flux during heat wave

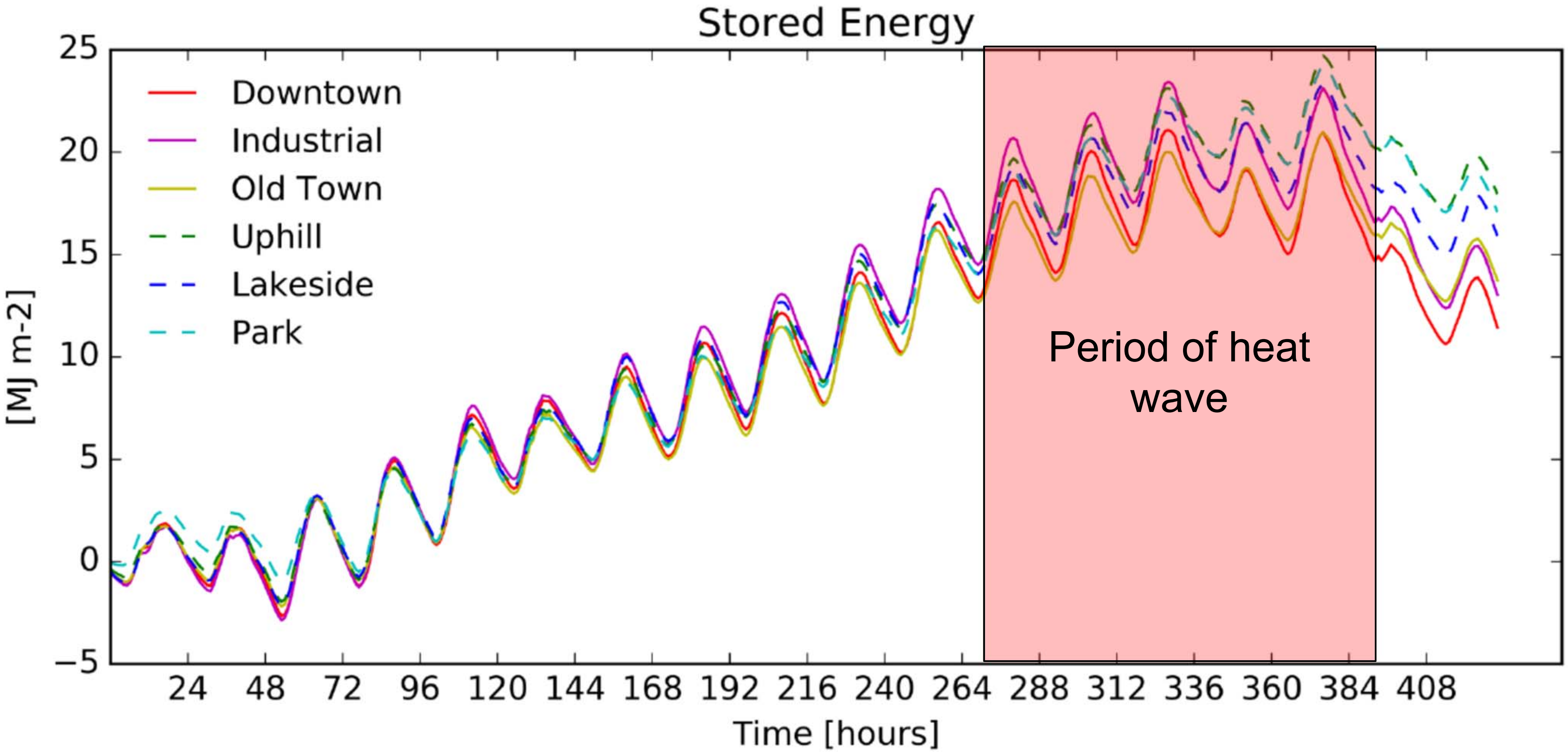
Res = 250 m

day

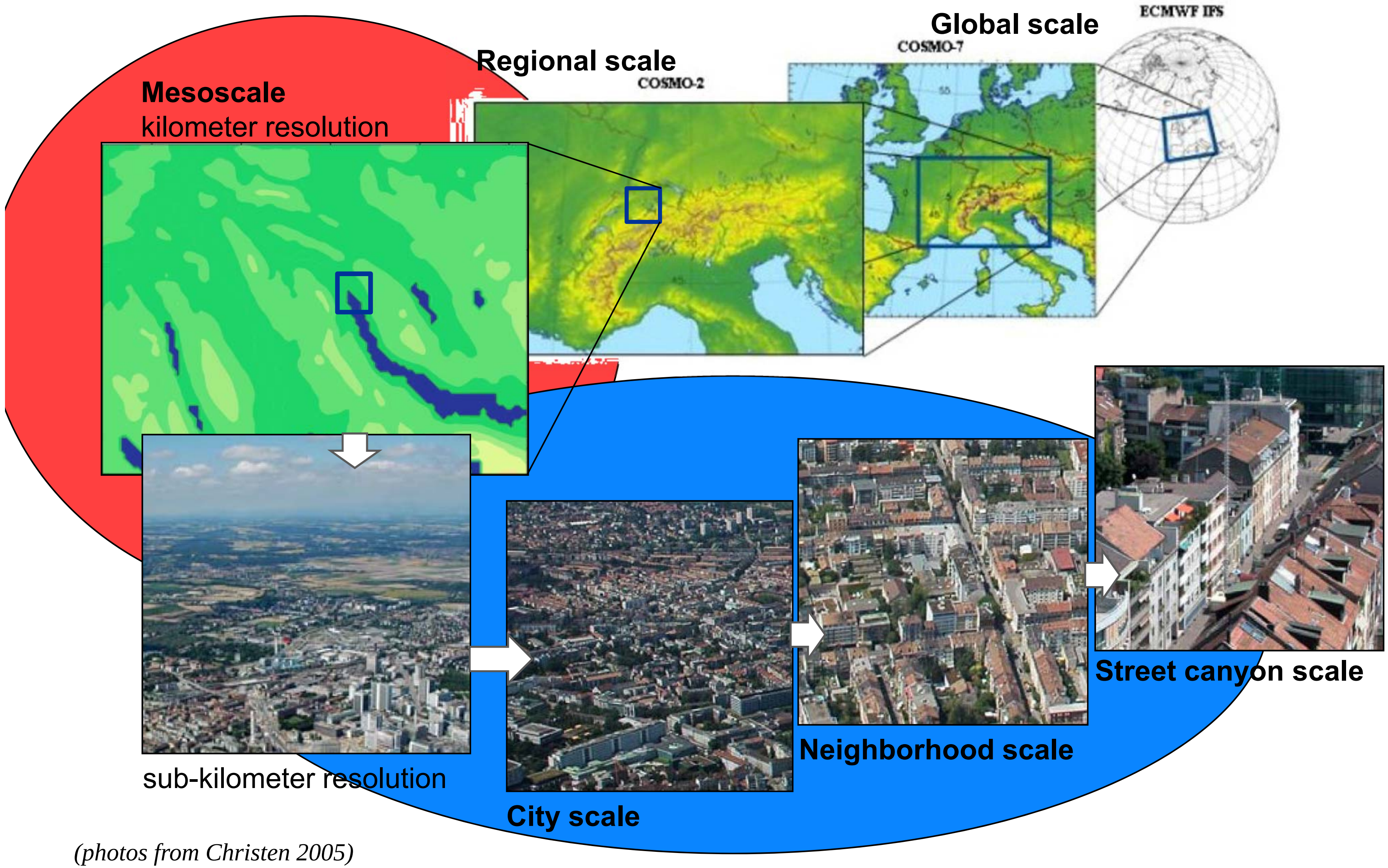
night



Heat Wave Analysis – simulated stored heat

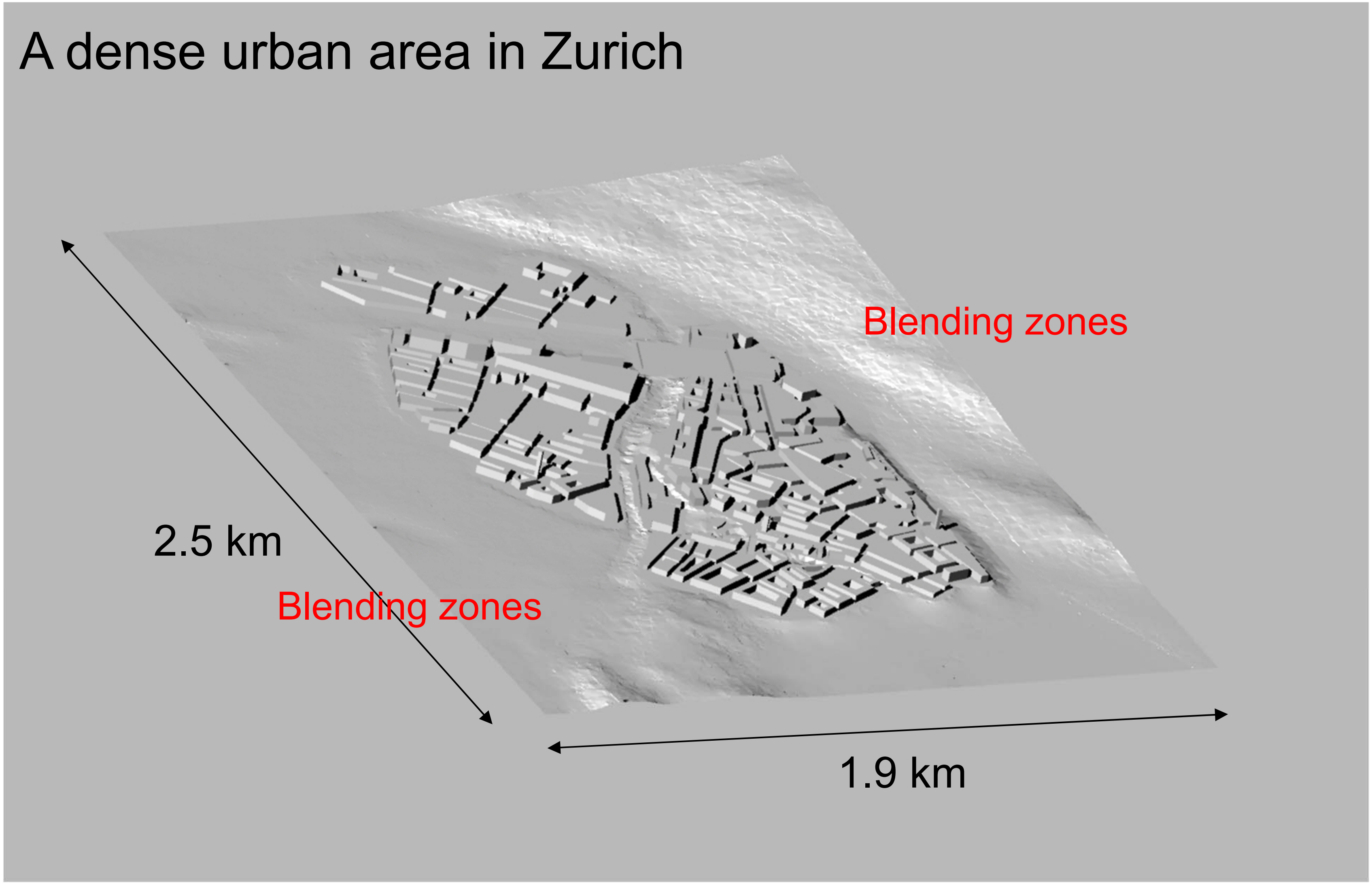


Linking mesoscale and city/neighborhood scale

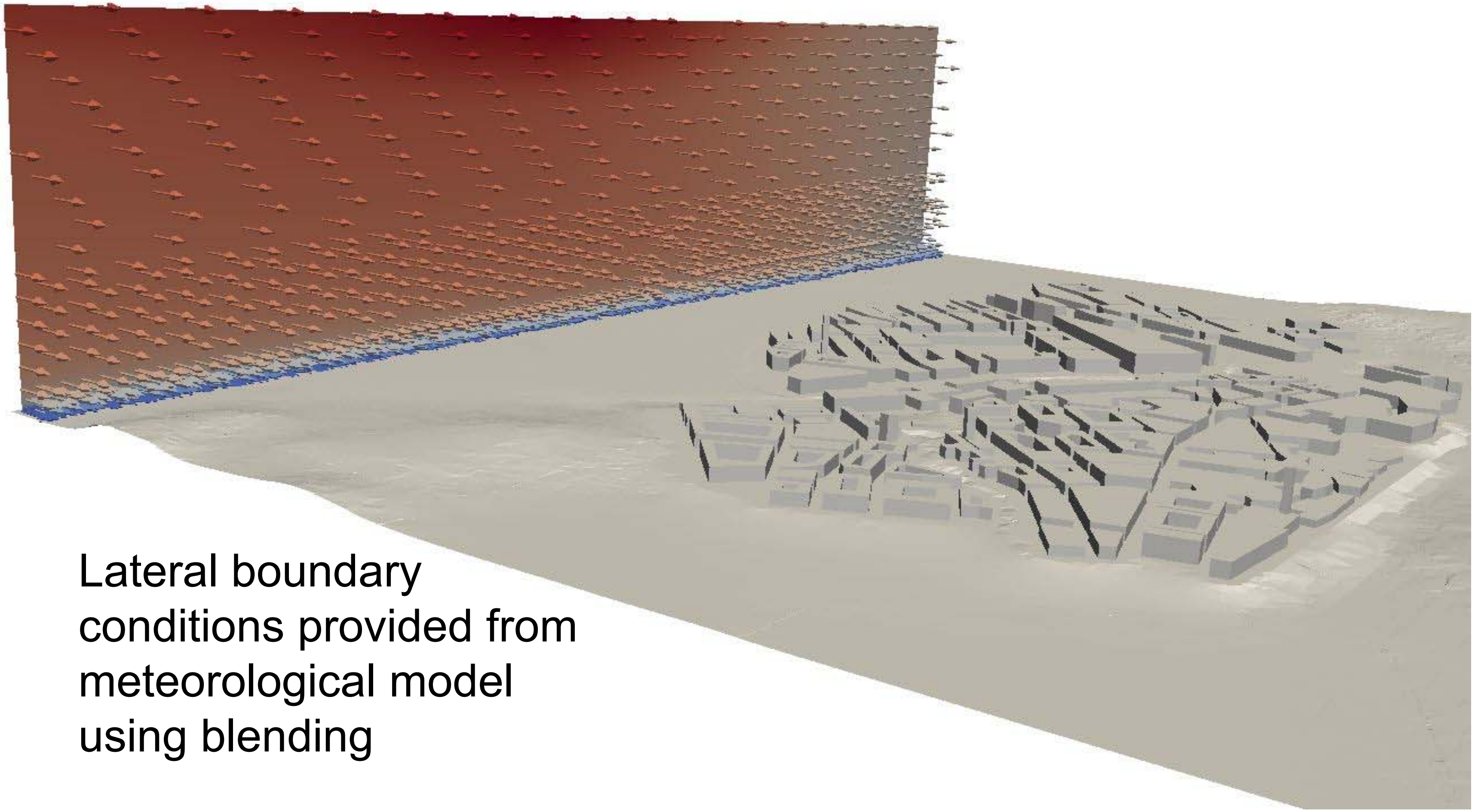


(photos from Christen 2005)

Building resolved city scale model



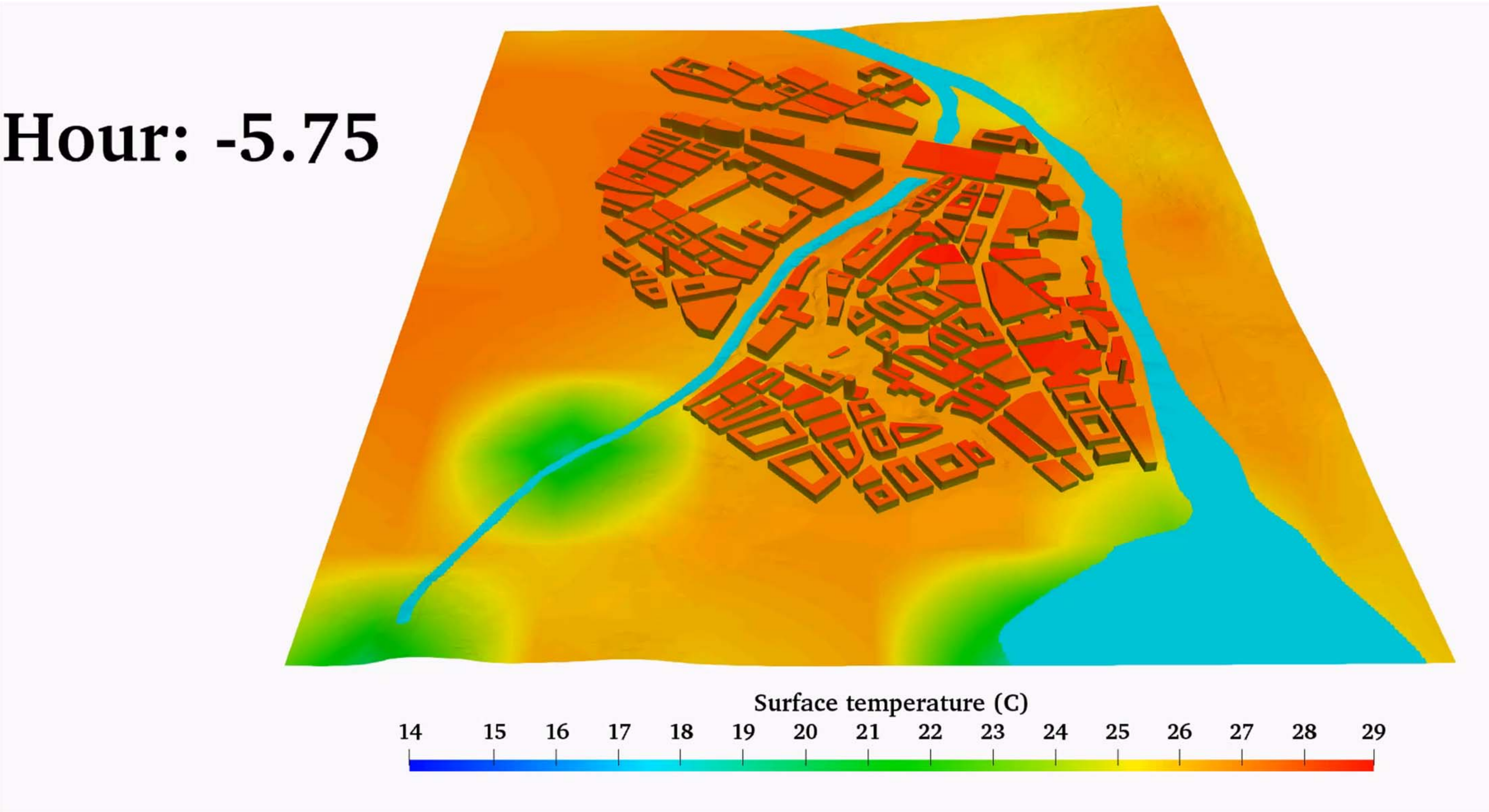
Boundary conditions: in- and outflow



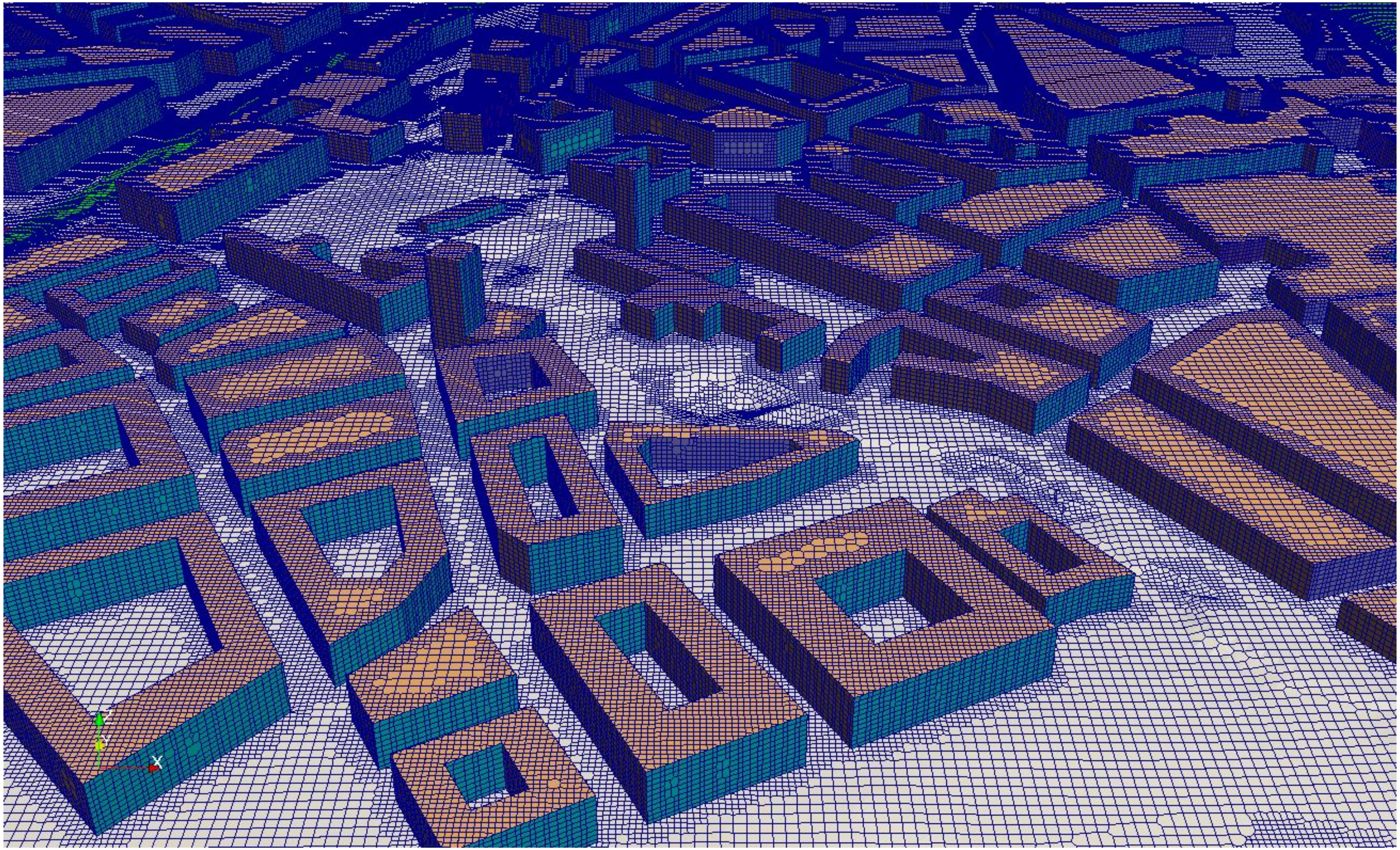
Lateral boundary
conditions provided from
meteorological model
using blending

Boundary conditions

Surface temperatures by downscaling from parametric model temperatures

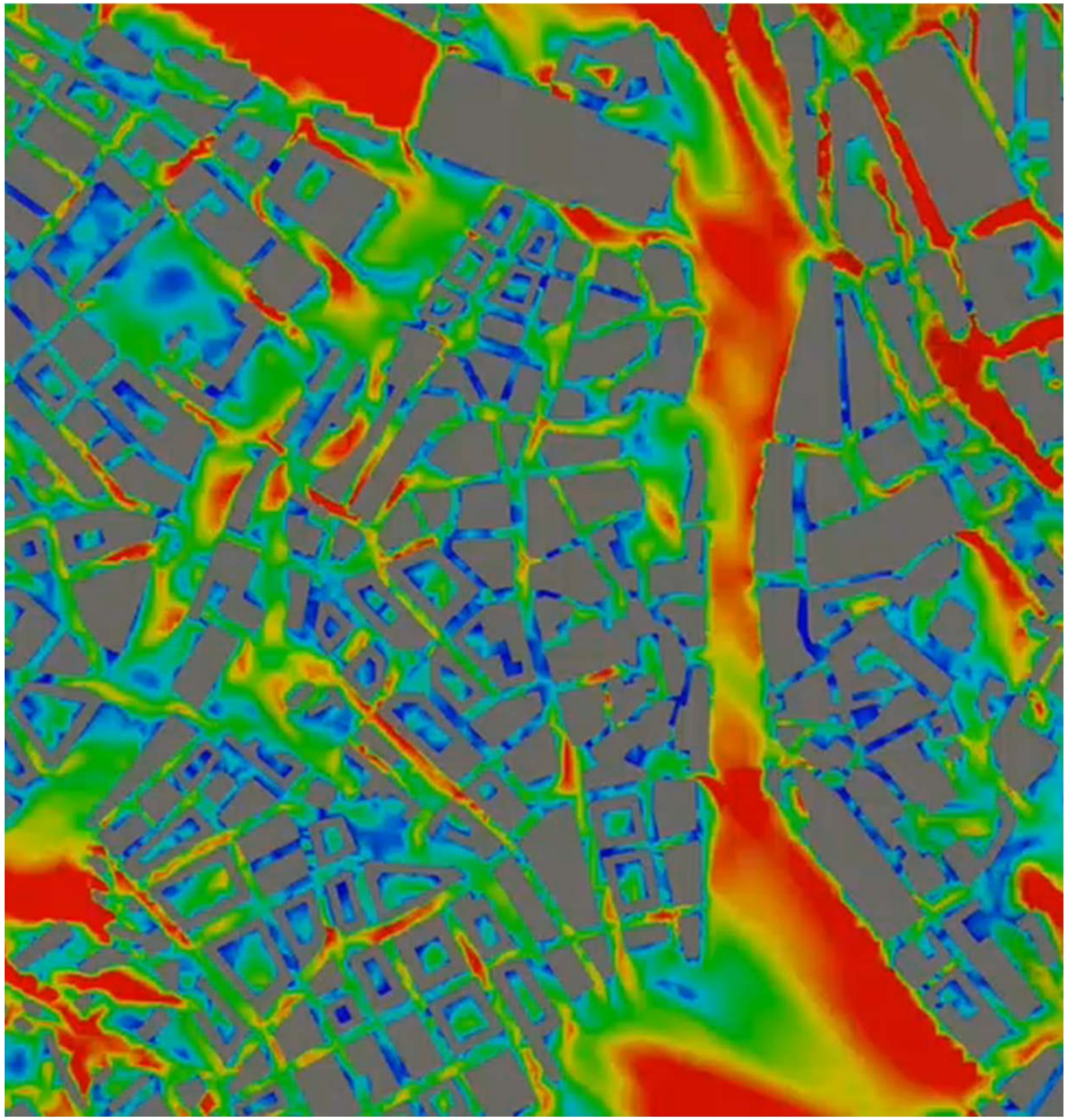


Building resolved city scale model

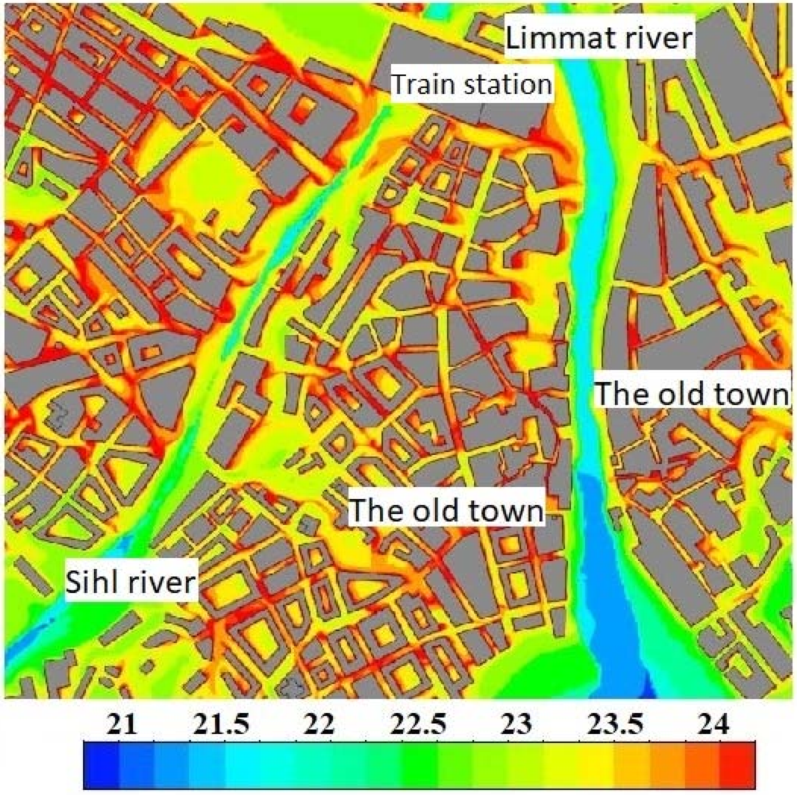


Mesh 3 million cells

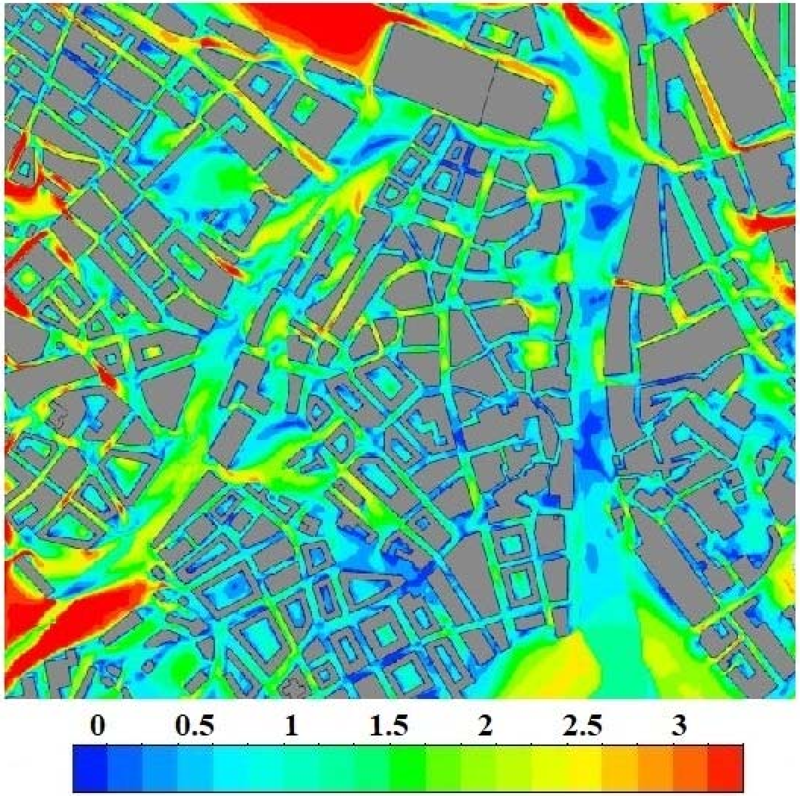
Wind speed at 2 m above the ground 24 hours in June 23, 2015, From midnight



Temperature and wind speed at 3 m

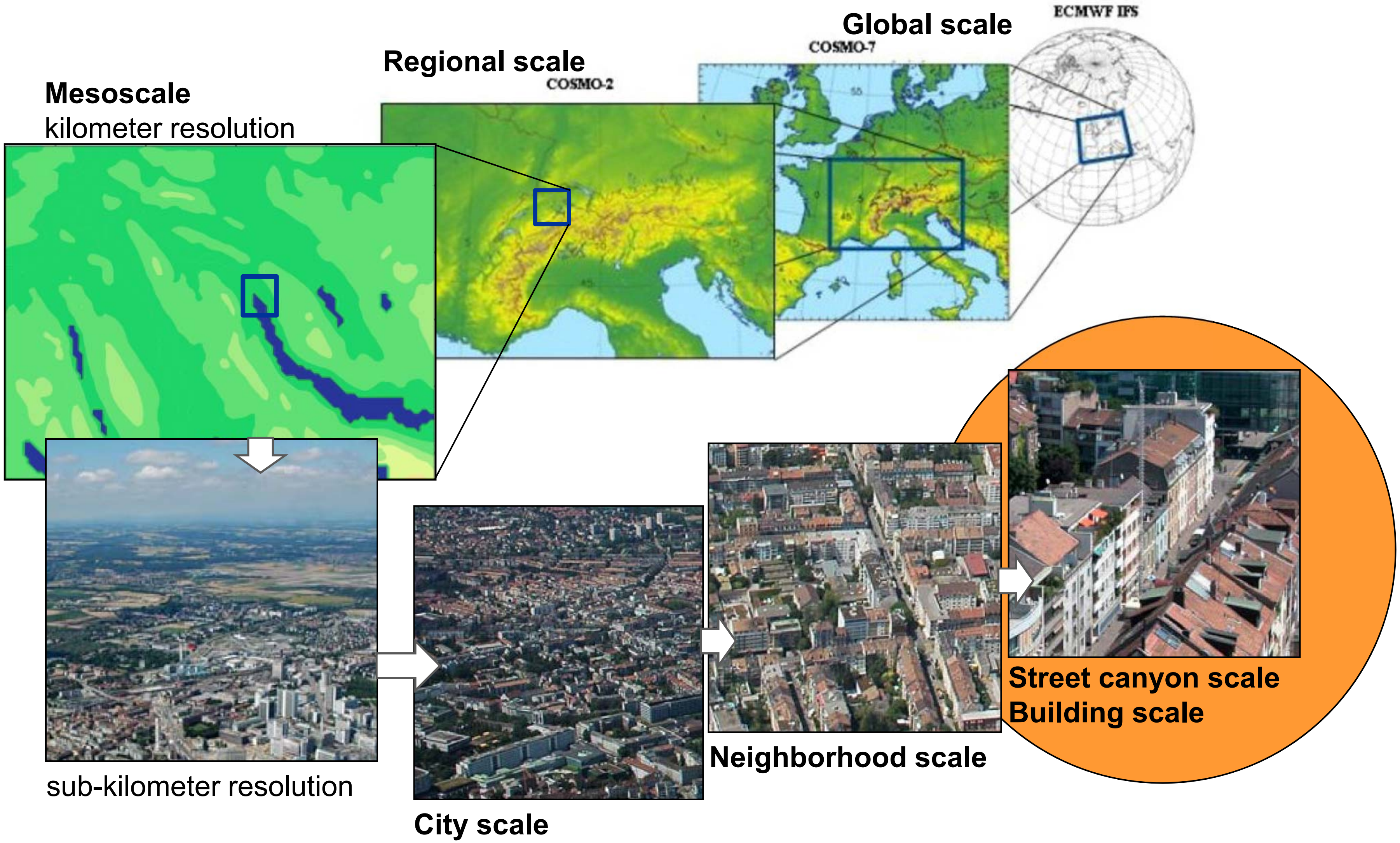


Temperature (C) at 3 m above the surface



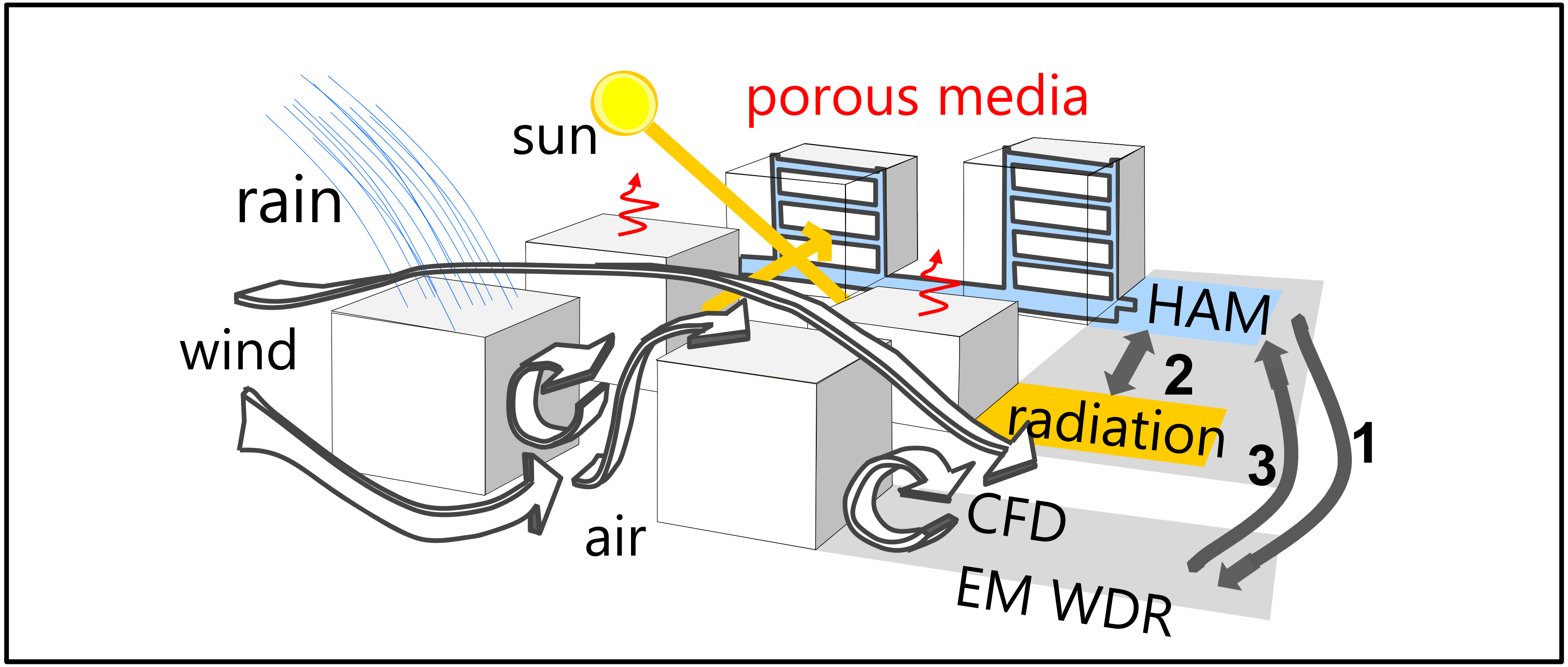
Wind speed (m/s) at 3 m above the surface

SCALE 3: Street canyon and building scale



(photos from Christen 2005)

Coupled model for urban climate



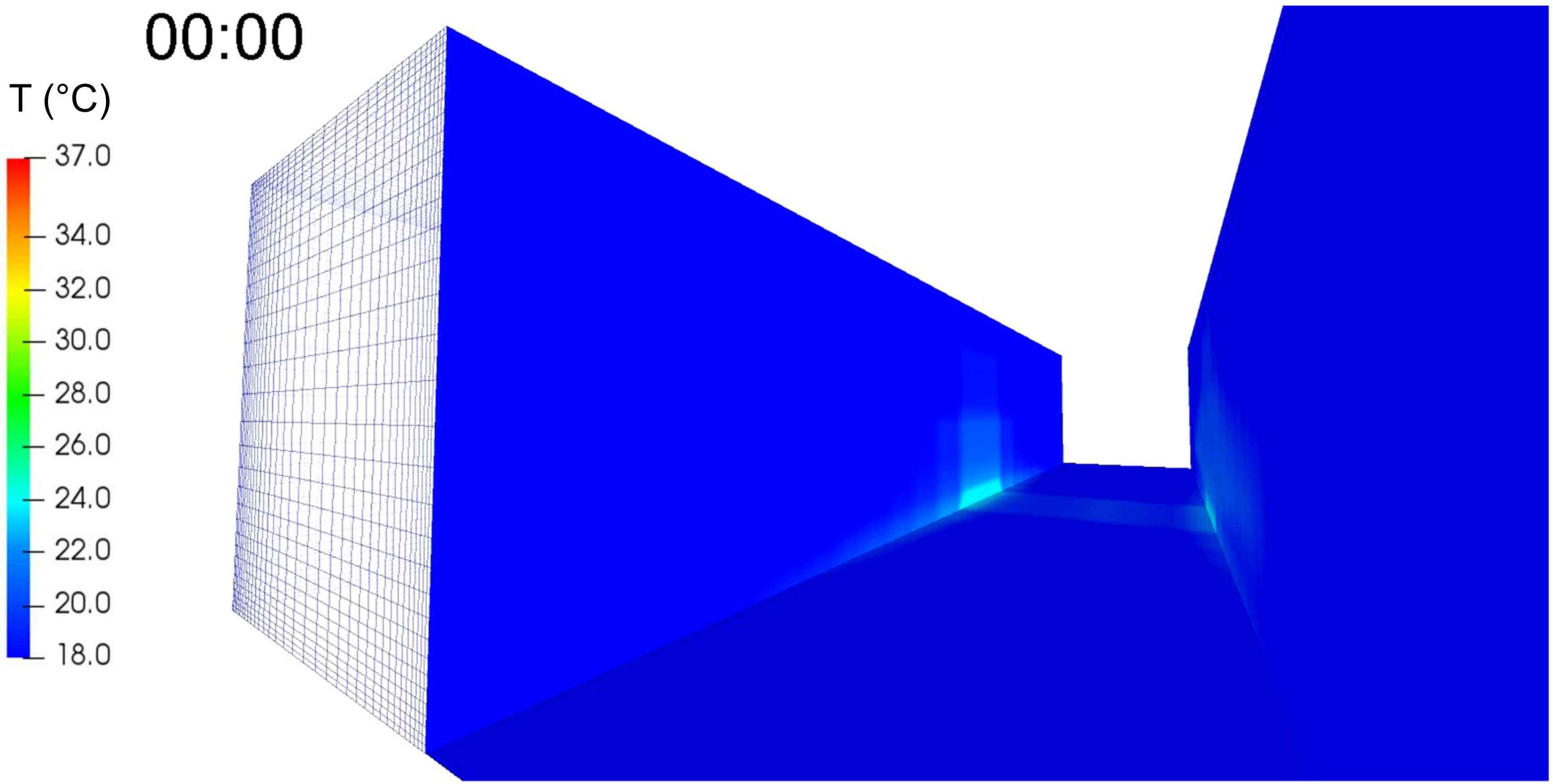
HAM **heat and moisture transport in porous materials (building materials, pavements, soils, …) including phase change: evaporative cooling**

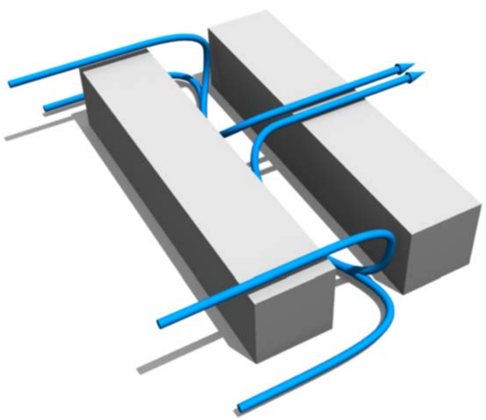
CFD air flow due to wind and buoyancy

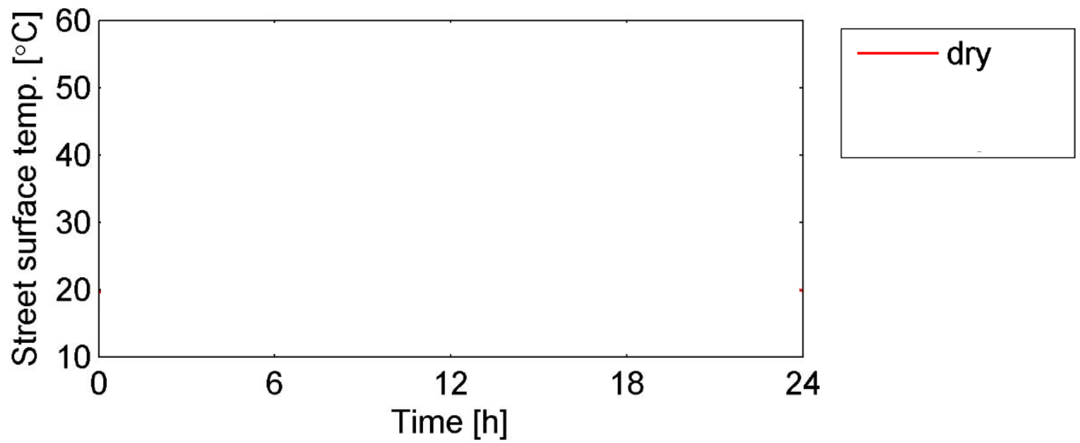
WDR wind driven rain, Eulerain multi-phase model

Radiation short and longwave radiation using view-factor method

Daily variation of surface temperature



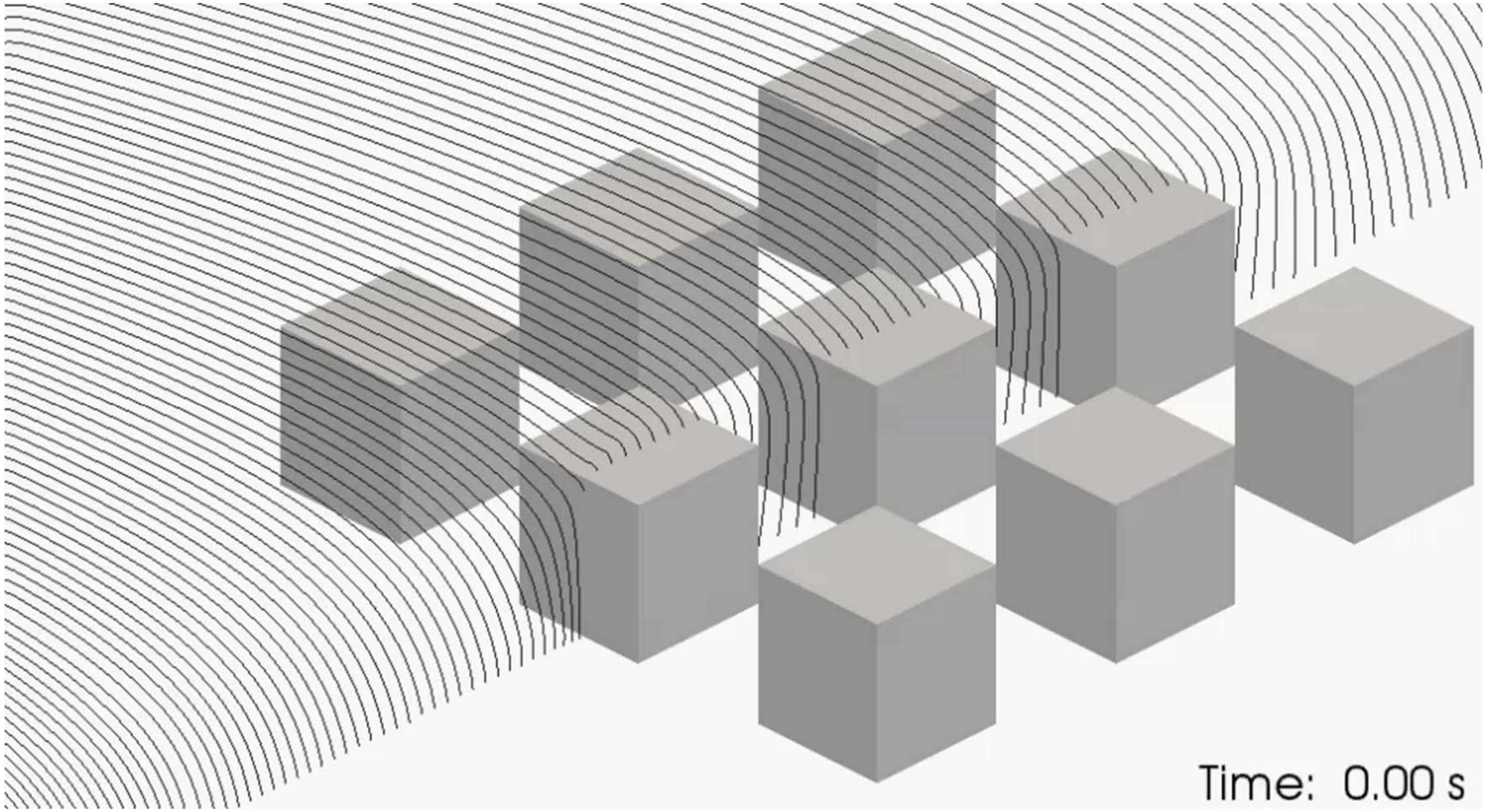




Eulerian Multiphase Numerical simulations
Wind Driven Rain with Large Eddy Simulation

Unsteady streamlines of rain phases

Droplet diameter = 0.3 mm, wind speed U = 1 m/s



Surface wetting due to wind-driven rain

Most important wetting of the street surface

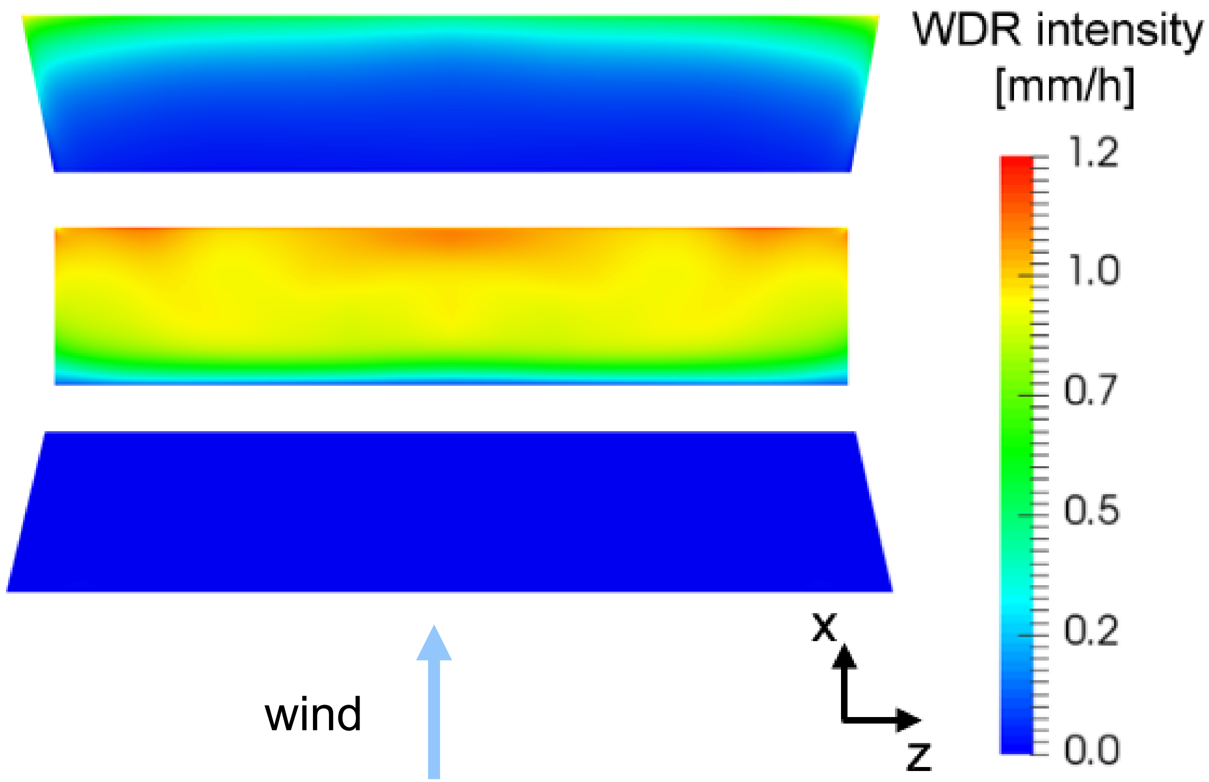
Surface-averaged

WDR intensity

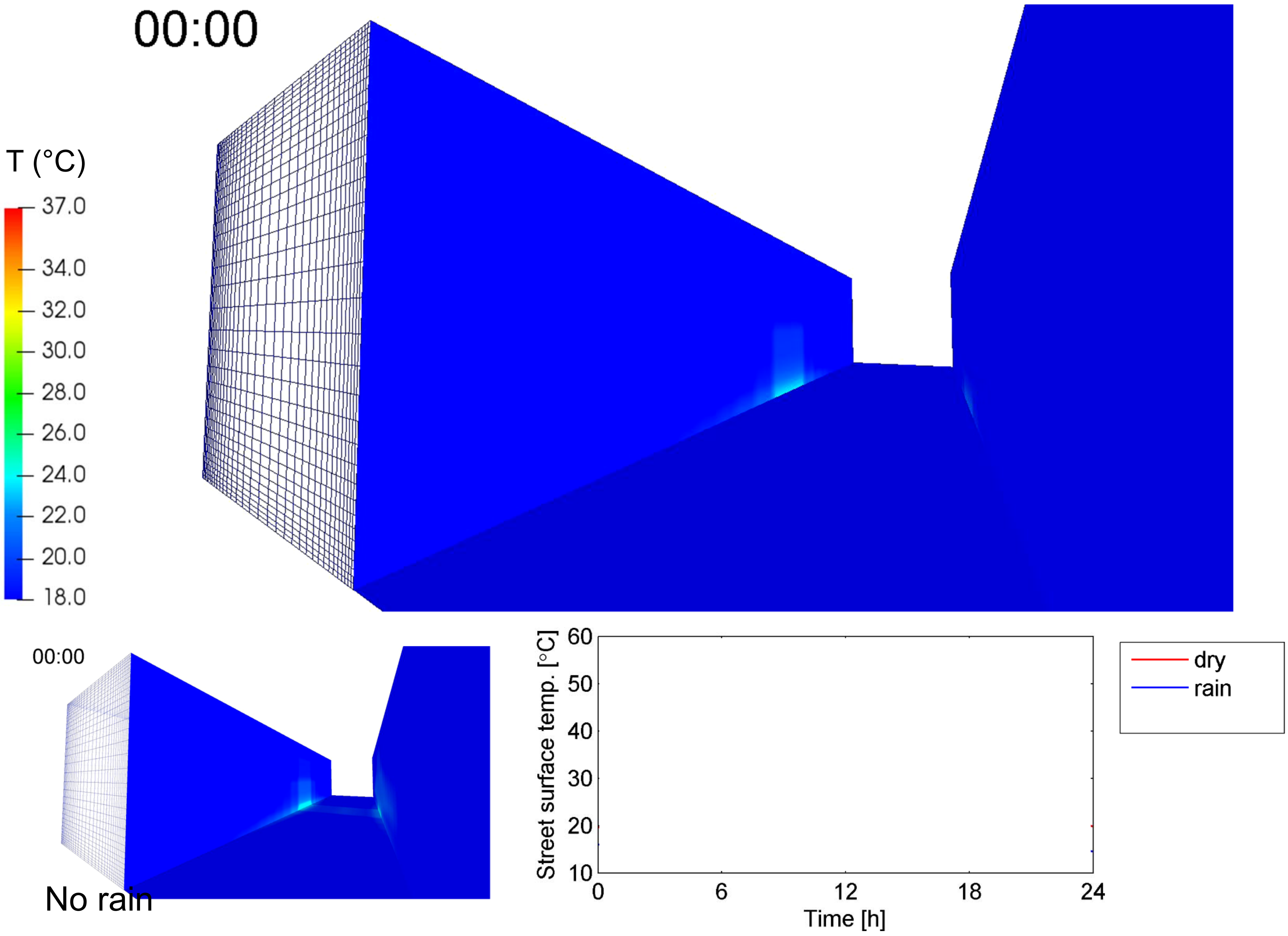
Leeward wall ≈ 0 mm/h

Street = 0.81 mm/h

Windward wall = 0.16 mm/h



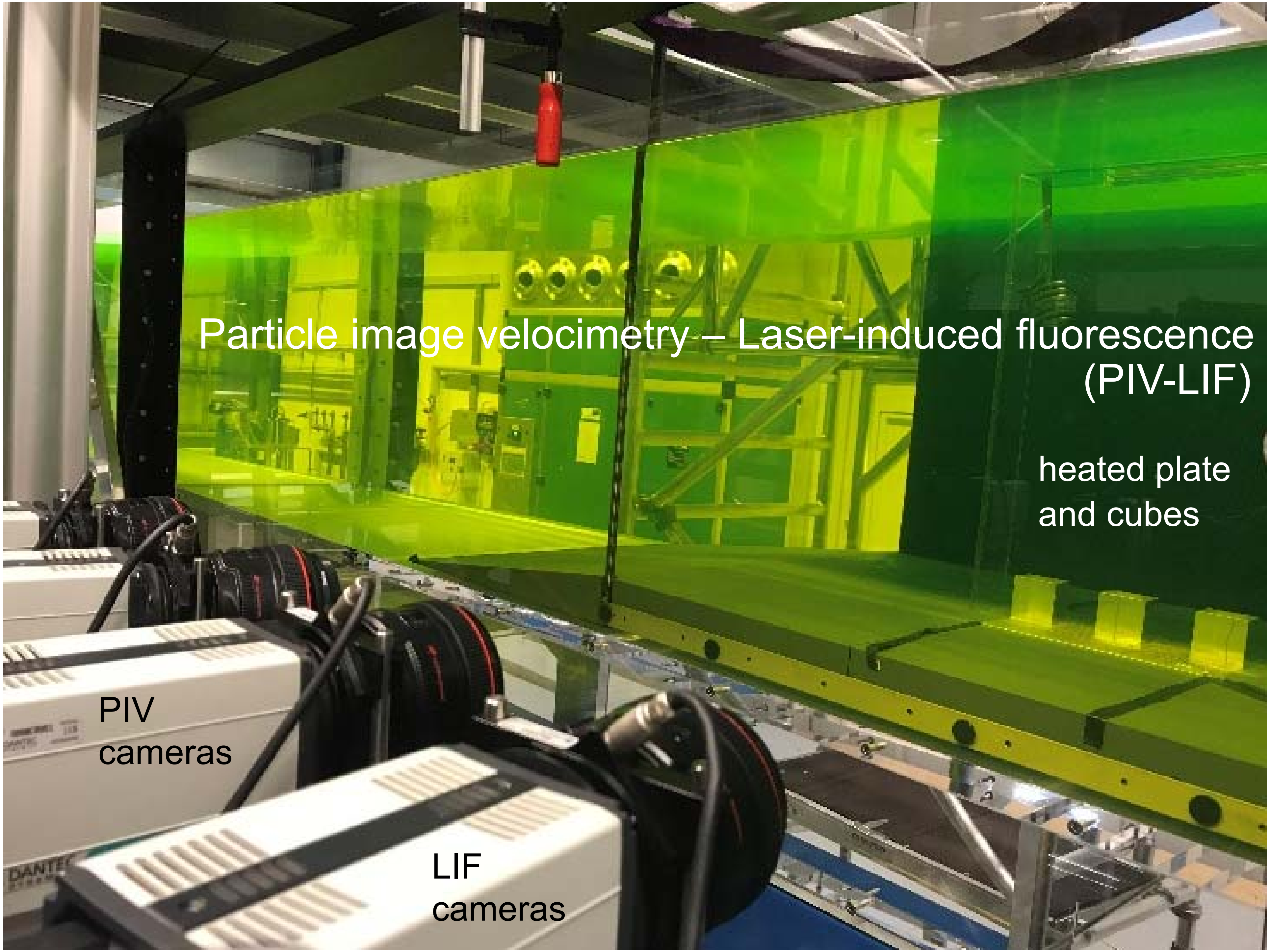
Daily variation of surface temperature **with rain**



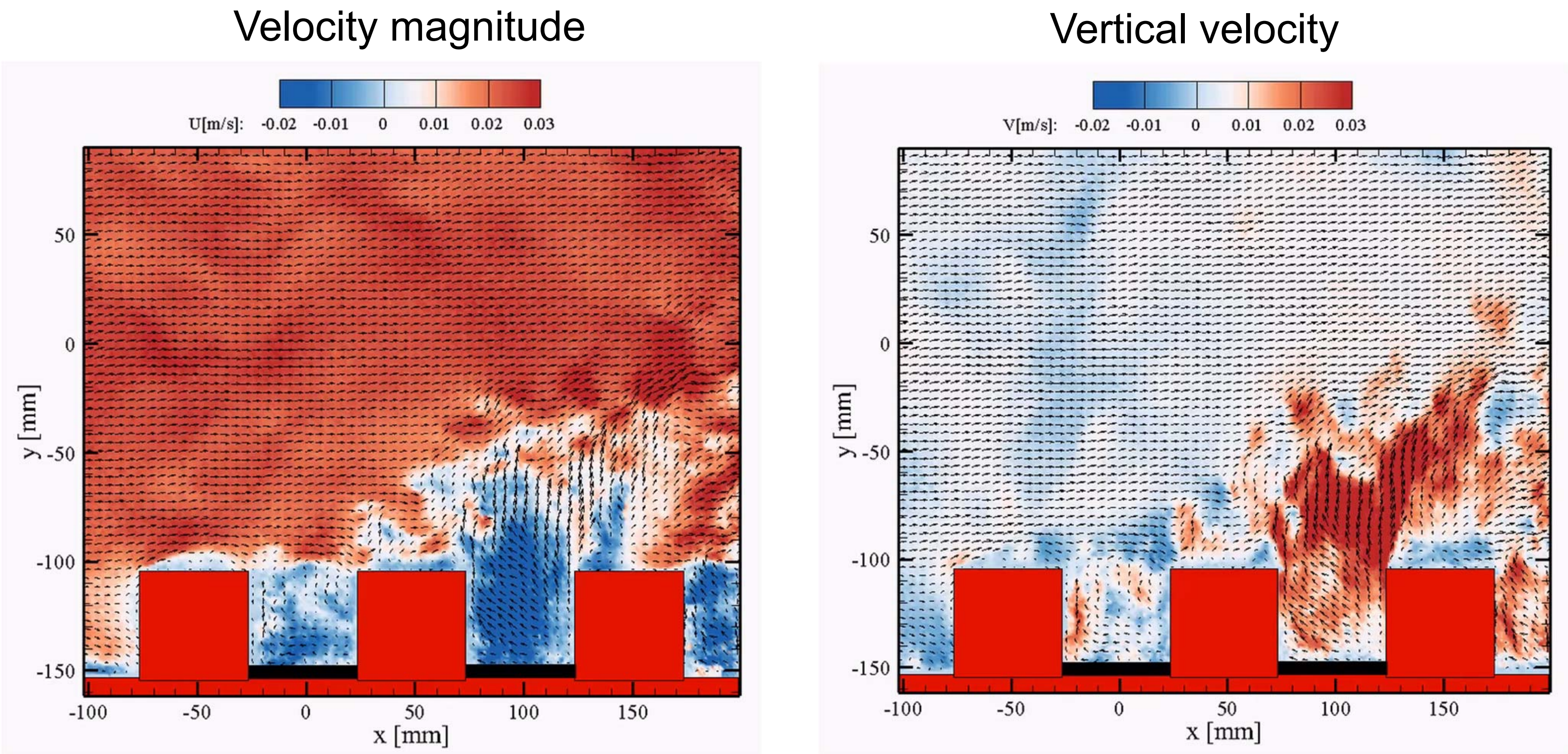
Multiscale models need

- validation of model on every scale

- validation of the links between the different scales


Particle image velocimetry – Laser-induced fluorescence
(PIV-LIF)
heated plate
and cubes
PIV
cameras
LIF
cameras

Time resolved PIV measurements, non-isothermal velocity field



Re: 1250, Ri: 4.39

Jiggar Shah, 2018

Questions

What is the impact of urban and local climate under climatic change on

- **Urban thermal comfort**, **heat stress,** health (pollutants)
- Building & urban (cooling) energy demand
- Hygrothermal performance and durability building envelopes

Evaluation of urban thermal comfort

Universal Thermal Climate Index (UTCI)

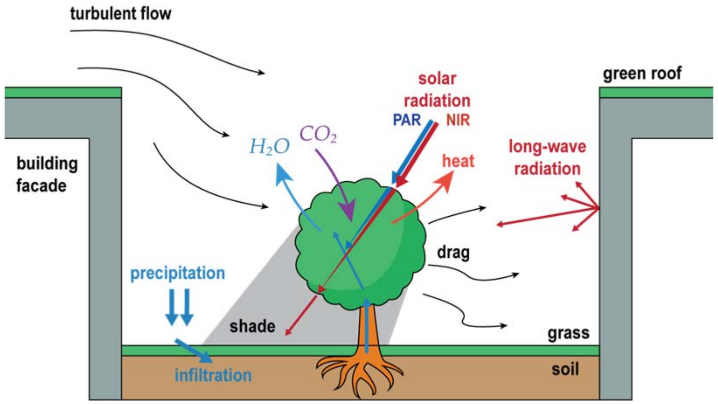
Equivalent ambient temperature of a reference environment providing the same physiological responses of a reference environment

- Air temperature
- Mean radiant temperature: surface temperature and solar radiation
- Relative humidity
- Wind speed
- Clothing
- Activity

UTCI range (ºC)	Stress category
> 46	Extreme heat stress (HS)
38 to 46	Very strong HS
32 to 38	Strong HS
26 to 32	Moderate HS
9 to 26	No thermal stress
0 to 9	Slight cold stress (CS)
-13 to 0	Moderate CS
-27 to -13	Strong CS
-40 to -27	Very strong CS
< -40	Extreme CS

Vegetation: shadowing and transpiration

Porous medium approach



Radiation model

+

Airflow model

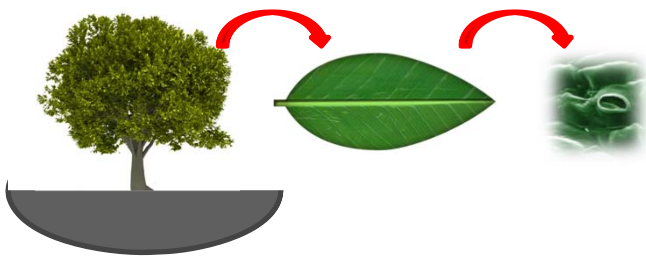
+

Vegetation model

+

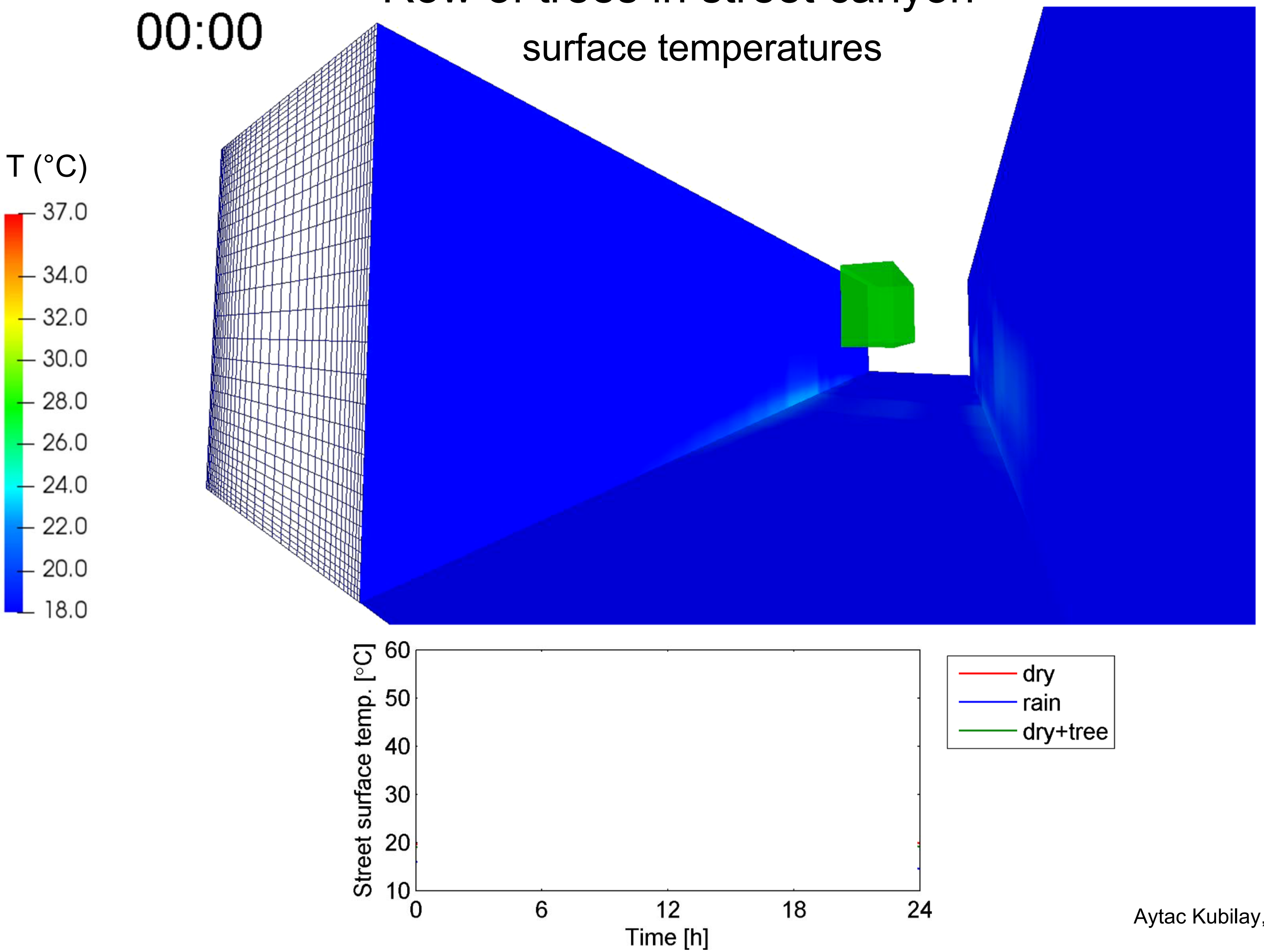
Soil model

Vegetation model : multiscale approach



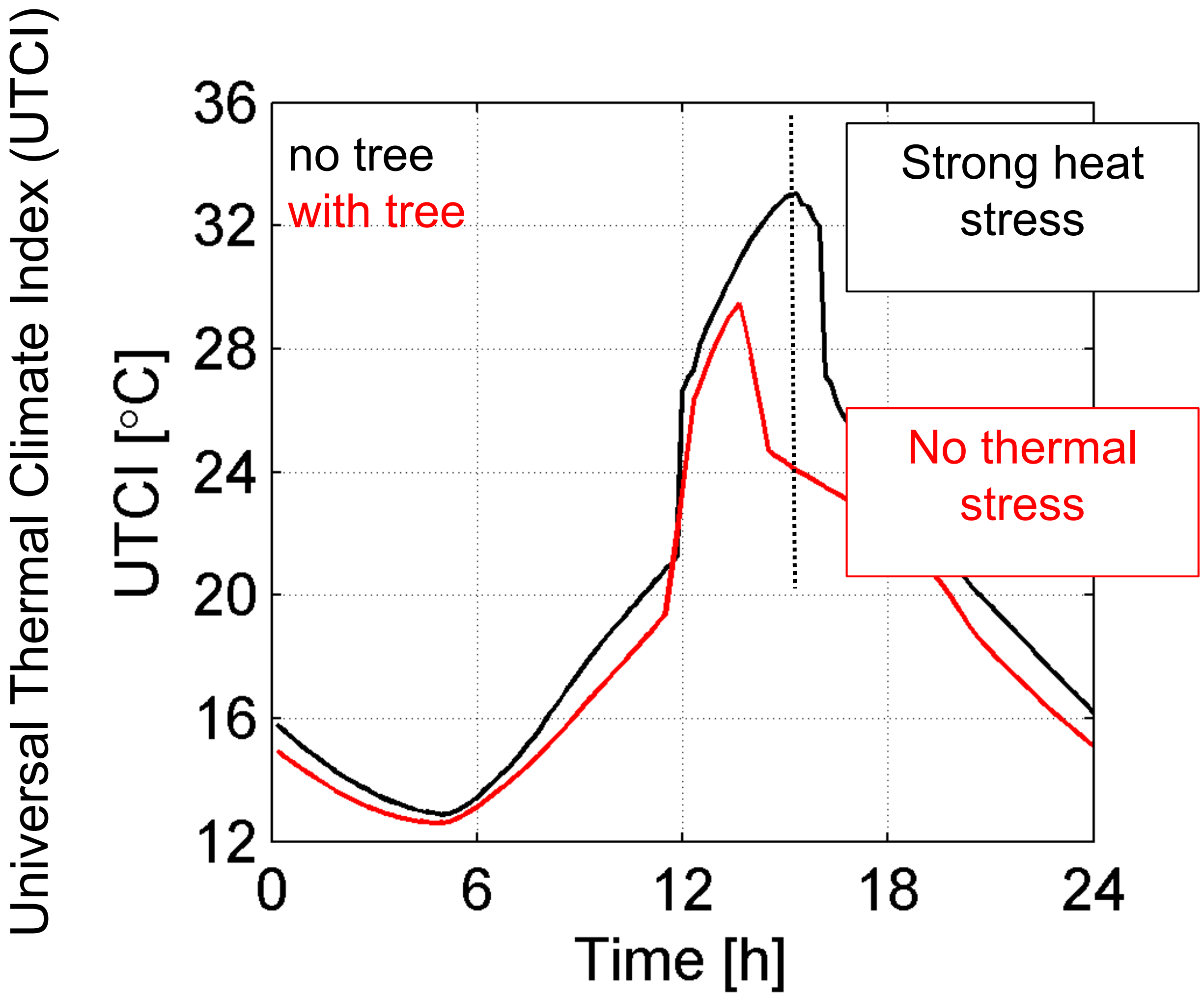
Row of trees in street canyon

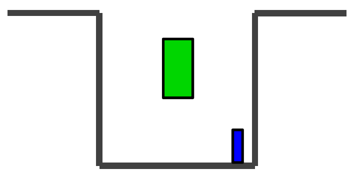
surface temperatures



Aytac Kubilay, 2017

Vegetation: shadowing and transpiration





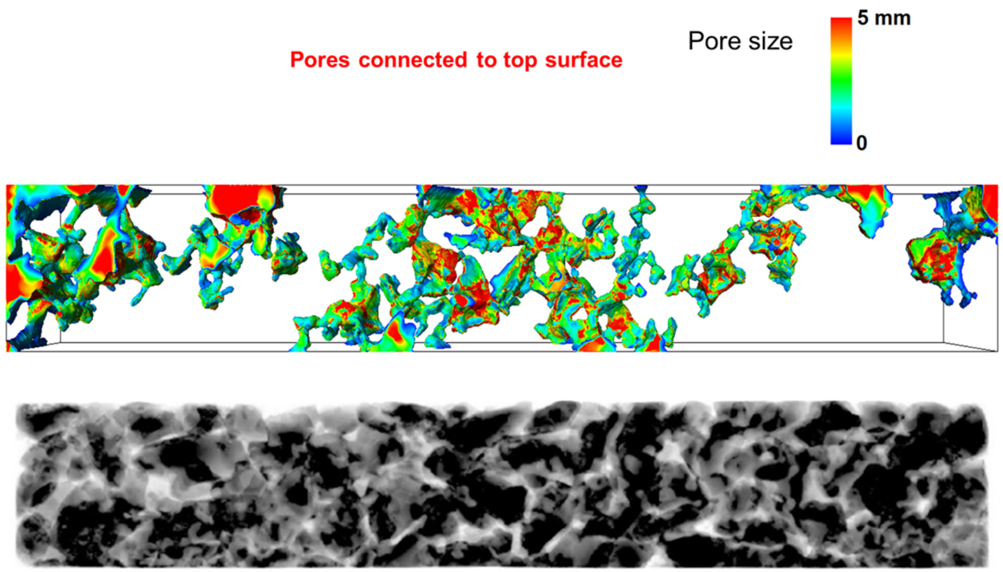
Tree is effective shadowing device that cools itself by transpiration

Evaporative cooling

Evaporative cooling by wetting of porous materials / pavements

Towards material scale

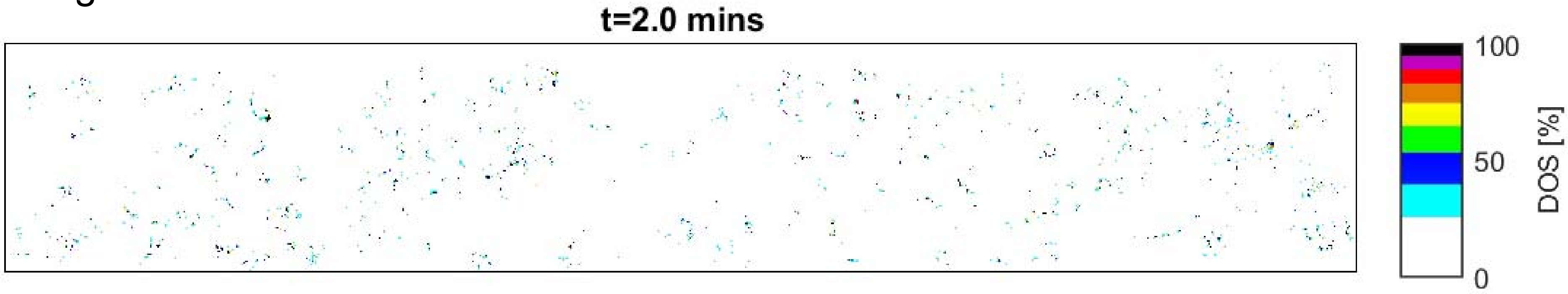
Can hydrophobic porous asphalts cool?



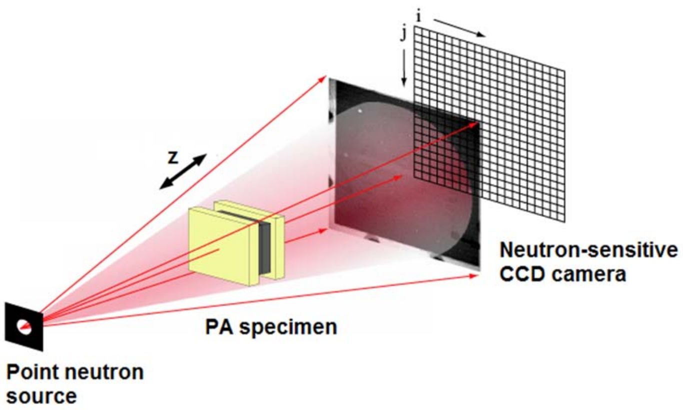
Understanding wetting by rain, drainage and drying

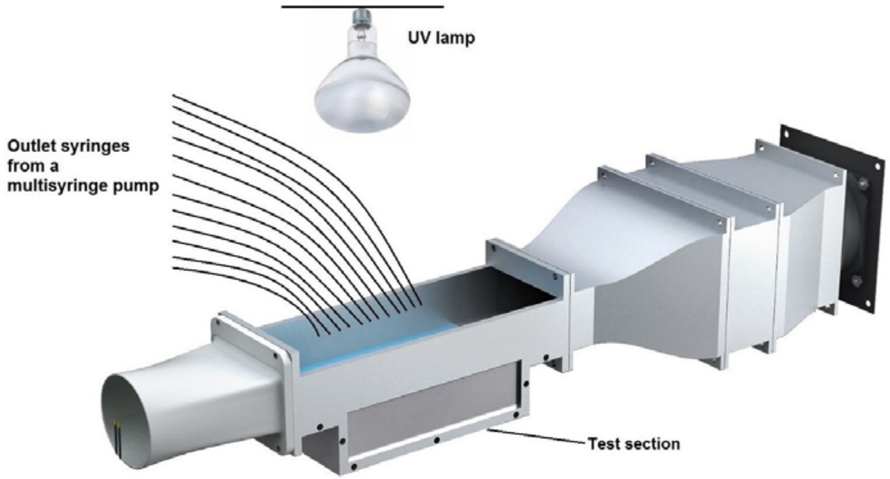
wetting by rain droplets of porous asphalt

Degree of saturation



Neutron radiography of wetting by rain in wind tunnel

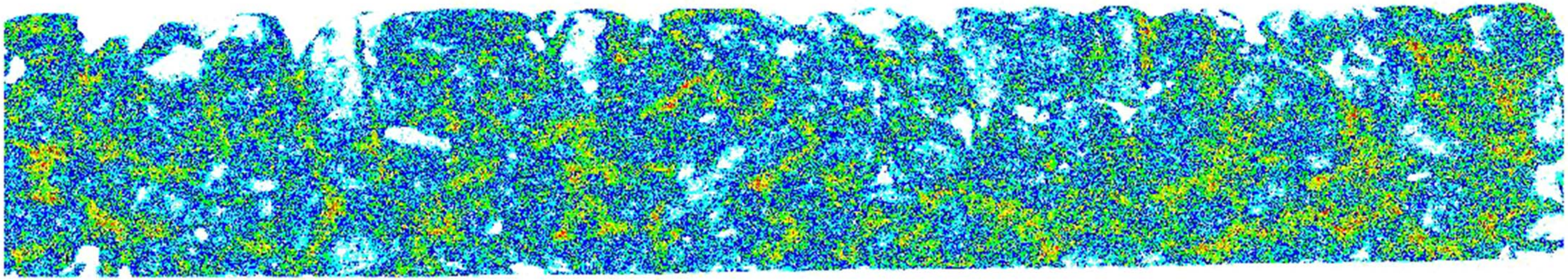




Study of wetting and drying by rain

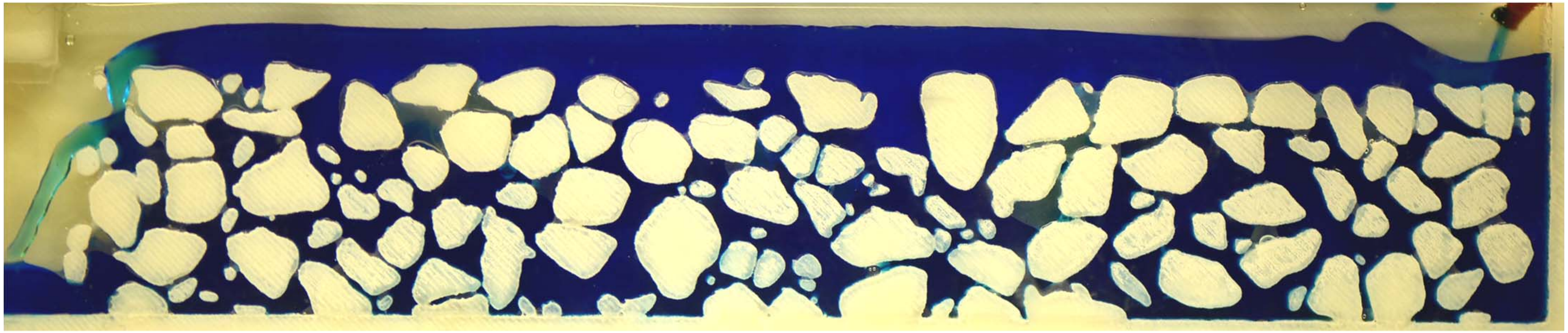
Neutron radiography

t = 1.0 mins

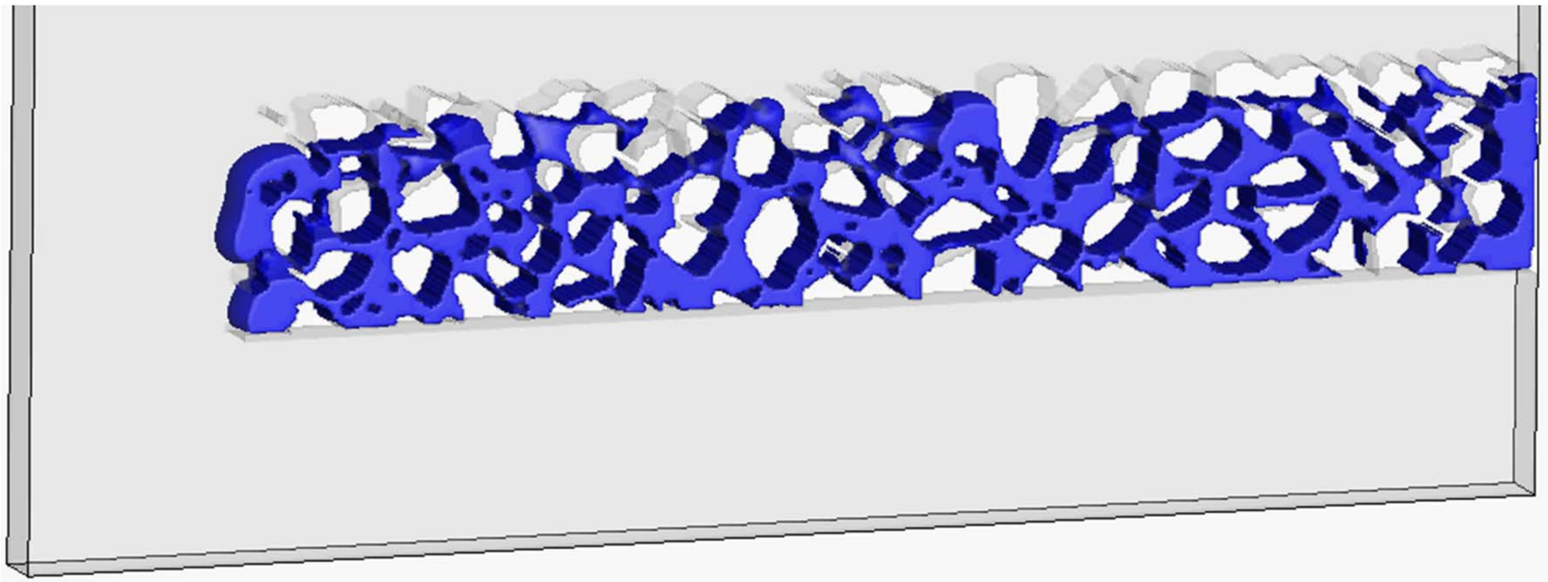


Study of drainage of water

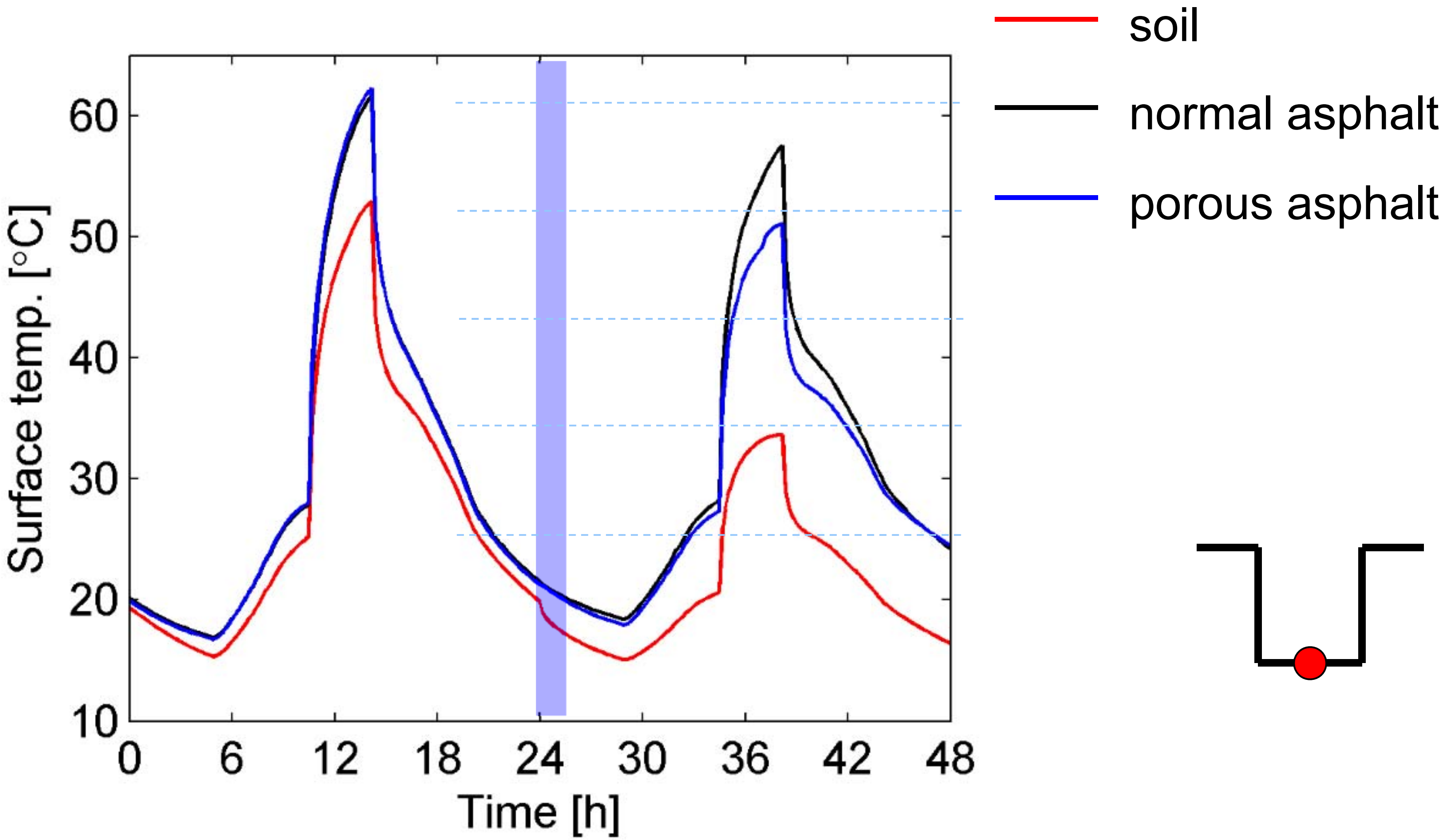
2D Microfluidic experiment



Lattice Boltzmann simulation (in house code)



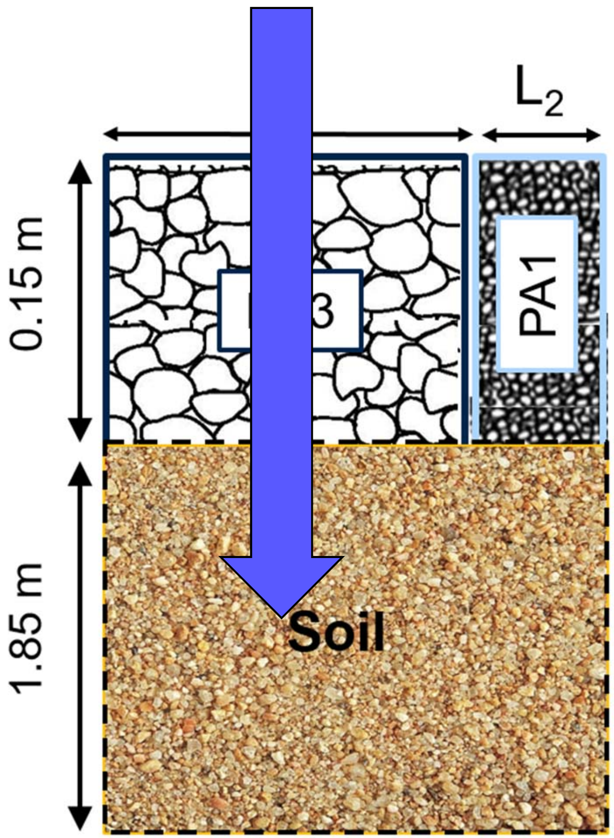
Evaporative cooling from porous asphalt



water is poured on street
reaching capillary saturation

How to optimize porous materials for evaporative cooling ?

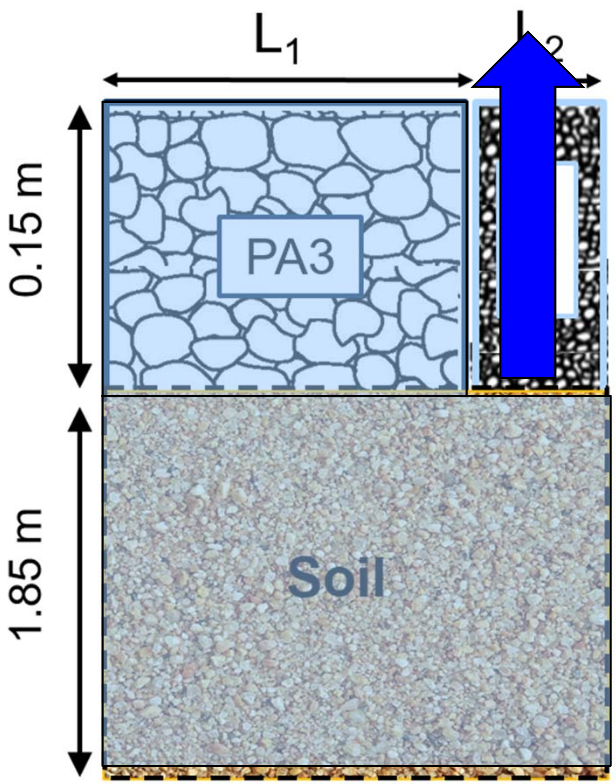
coarse pore part (PA3) drains and stores rain water



How to optimize porous materials for evaporative cooling ?

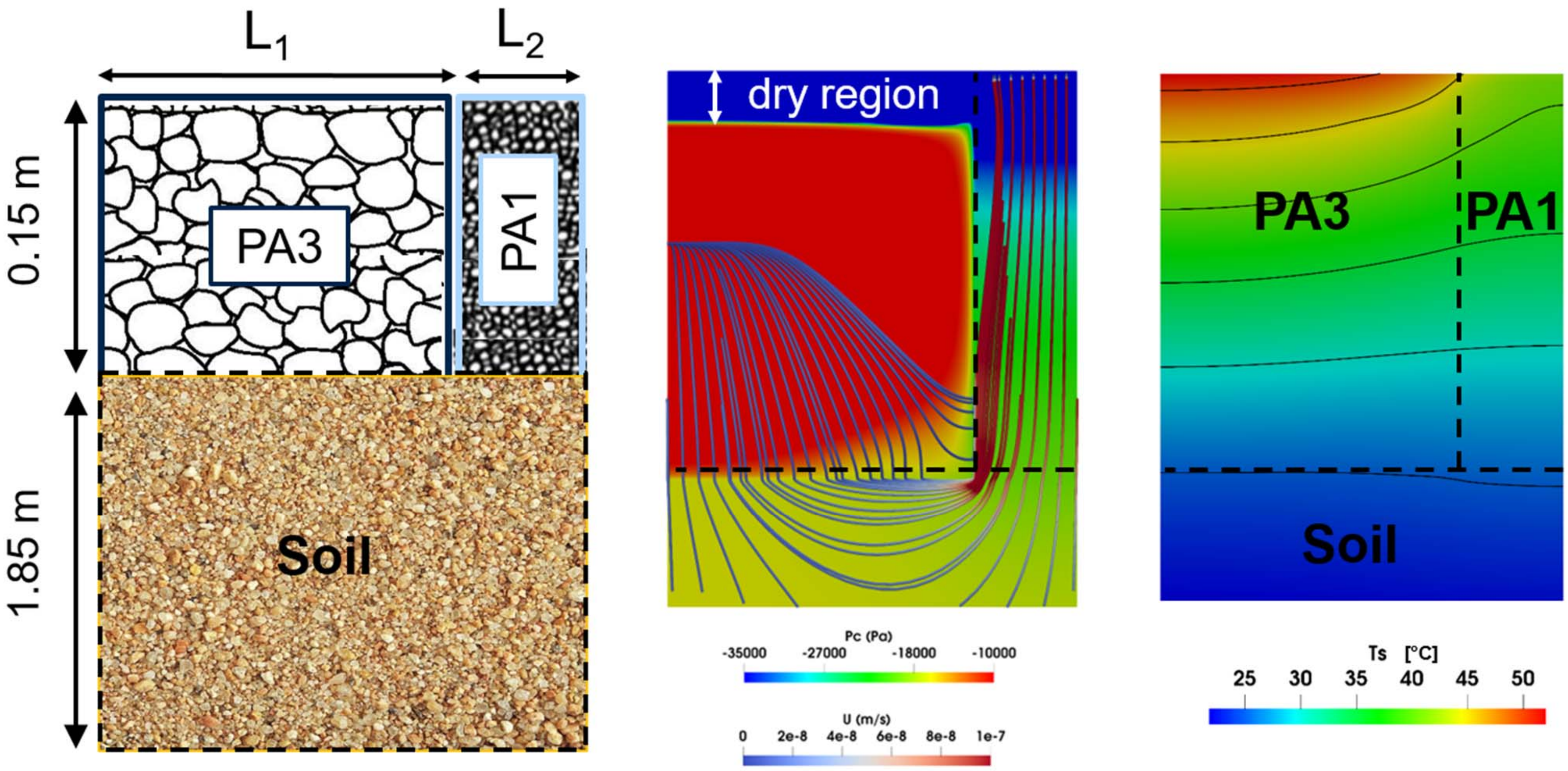
coarse pore part (PA3) drains and stores rain water

Fines pore part (PA1) sucks up the water for evaporative cooling



How to optimize porous materials for evaporative cooling ?

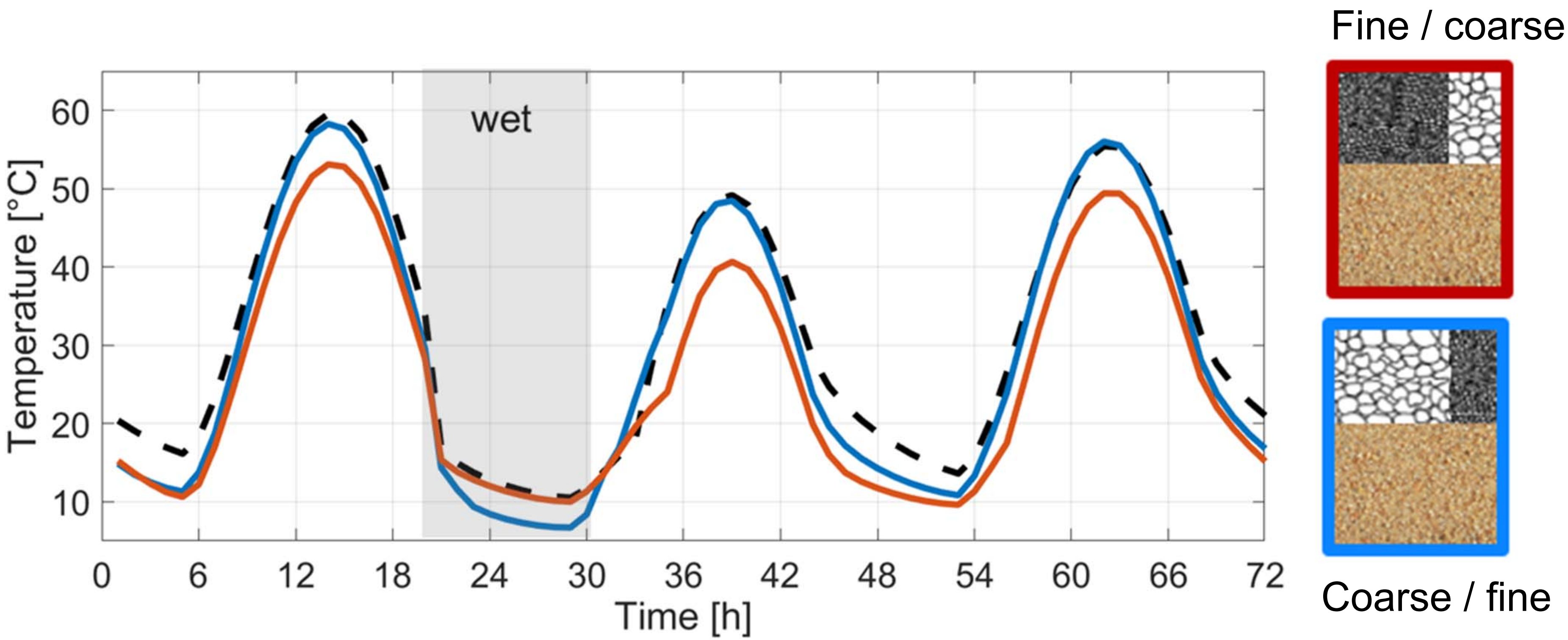
2 dimensional simulation



How to optimize porous materials for evaporative cooling ?

Red configuration works

Blue configuration does not work



Connected presentations:

Integrated vegetation model for studying the cooling potential of trees in urban street canyons, **Tuesday 10:45 AM**, **Aytac Kubilay**

Using rain and vegetation to improve thermal comfort in a hot street canyon with fully-integrated urban climate modeling, **Tuesday 11:00 AM**, **Aytac Kubilay**

Questions

What is the impact of urban and local climate under climatic change on

- Urban thermal comfort, heat stress, health (pollutants)
- **Building & urban (cooling) energy demand**
- Hygrothermal performance and durability building envelopes

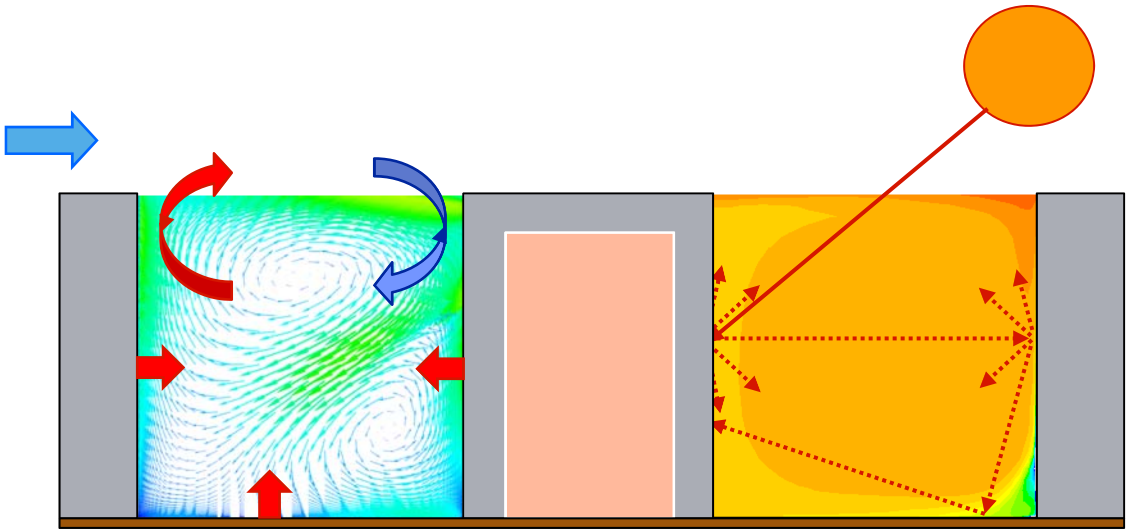
Building Cooling

Current building energy models do not take into account

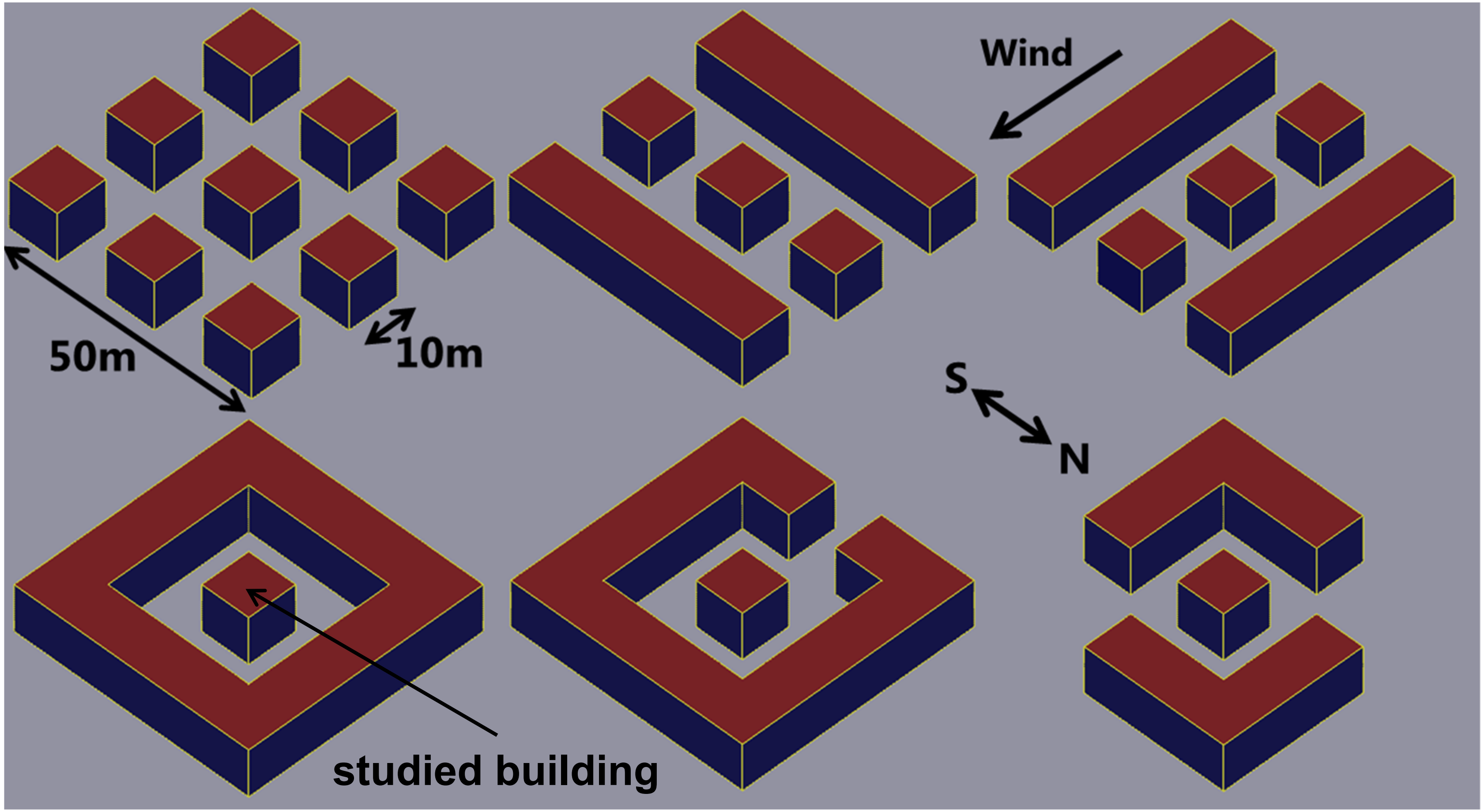
local urban climate

Three phenomena

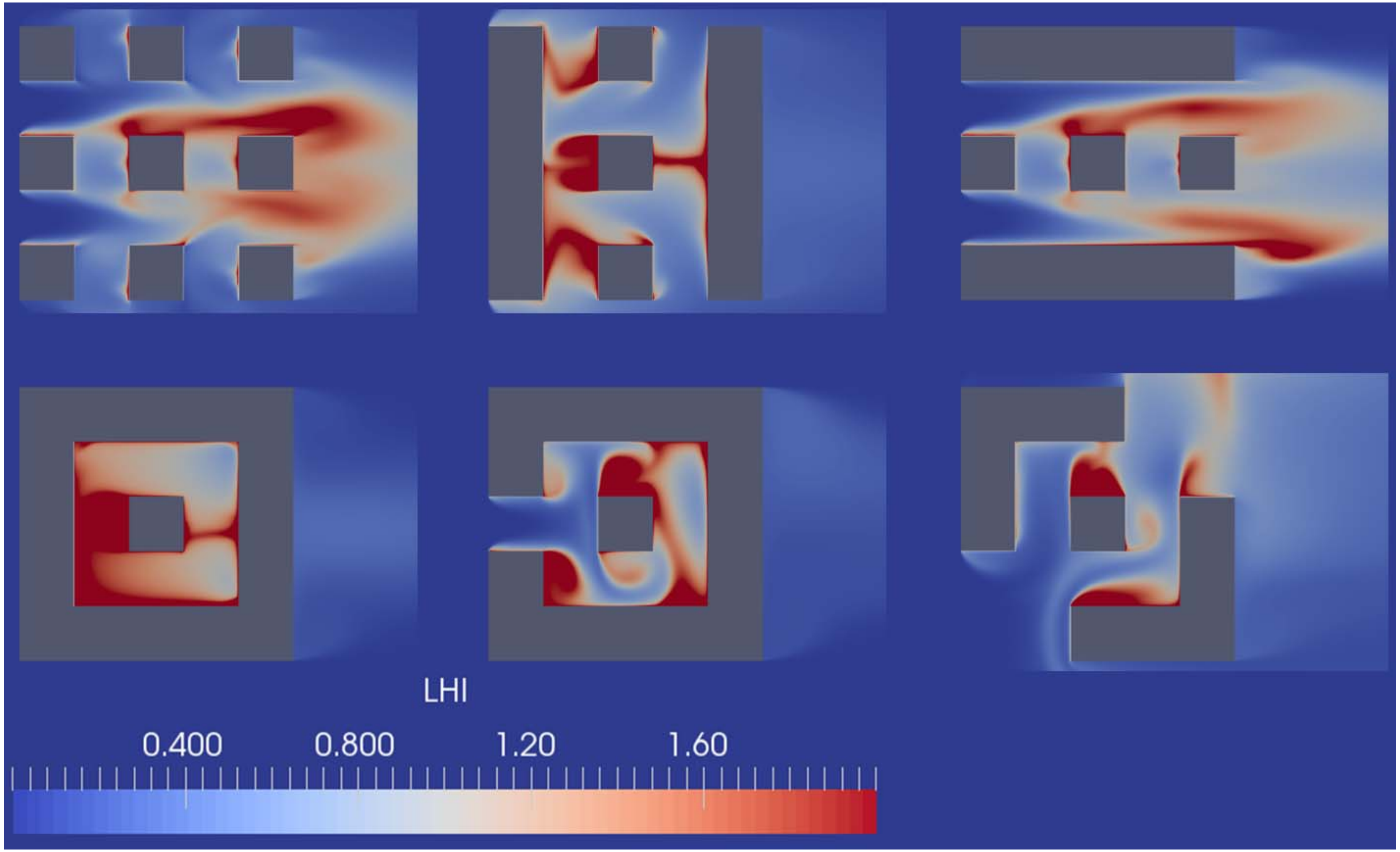
- Radiation: entrapment of shortwave/longwave radiation between buildings due to multiple reflections: higher surface temperatures
- Lower convective heat transfer coefficients due to sheltering
- Higher air temperatures due to global and local heat islands



Building cooling demand for central building
in different urban contexts

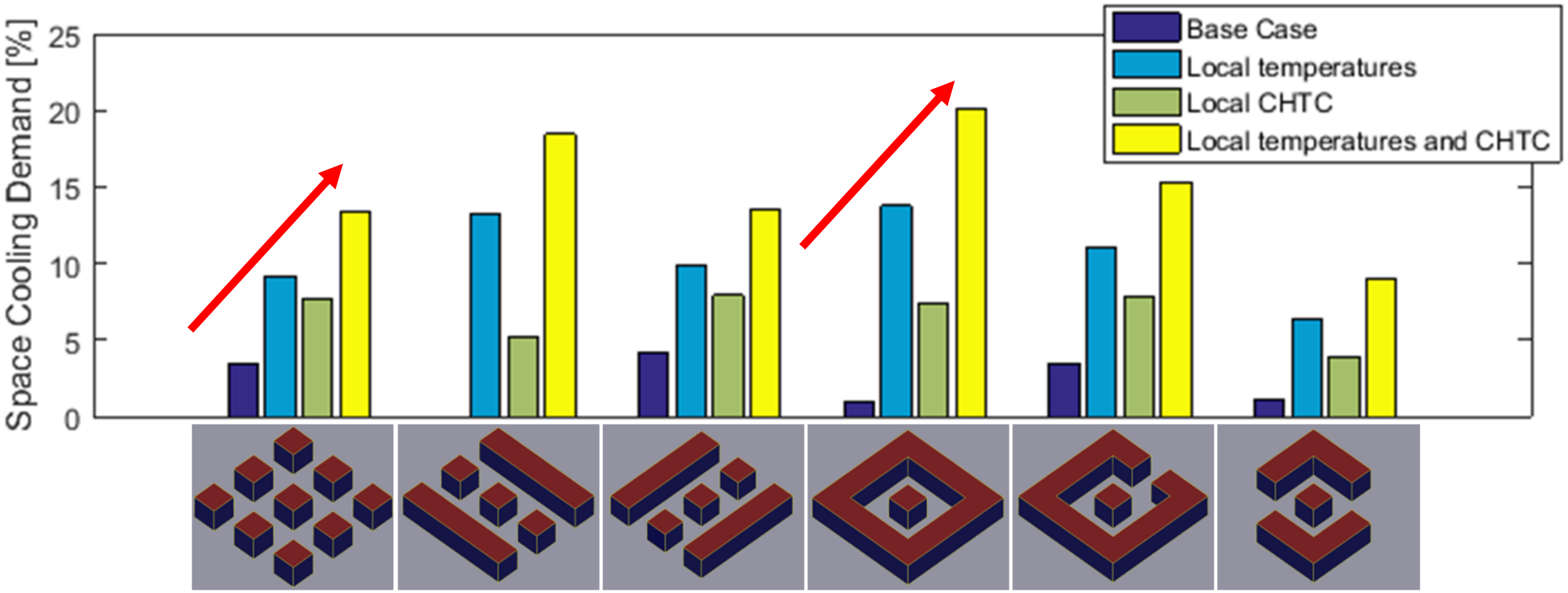


Local heat island intensity for central building in different urban contexts



Heat wave conditions in Zurich, office buildings, 4 pm

Building cooling demand for central building in different urban contexts



a) Base case: business as usual

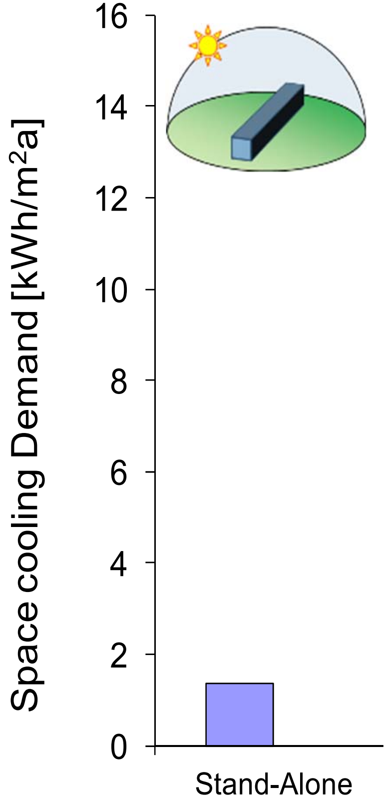
b) Local (intake) air temperatures

c) Local convective heat transfer coefficients

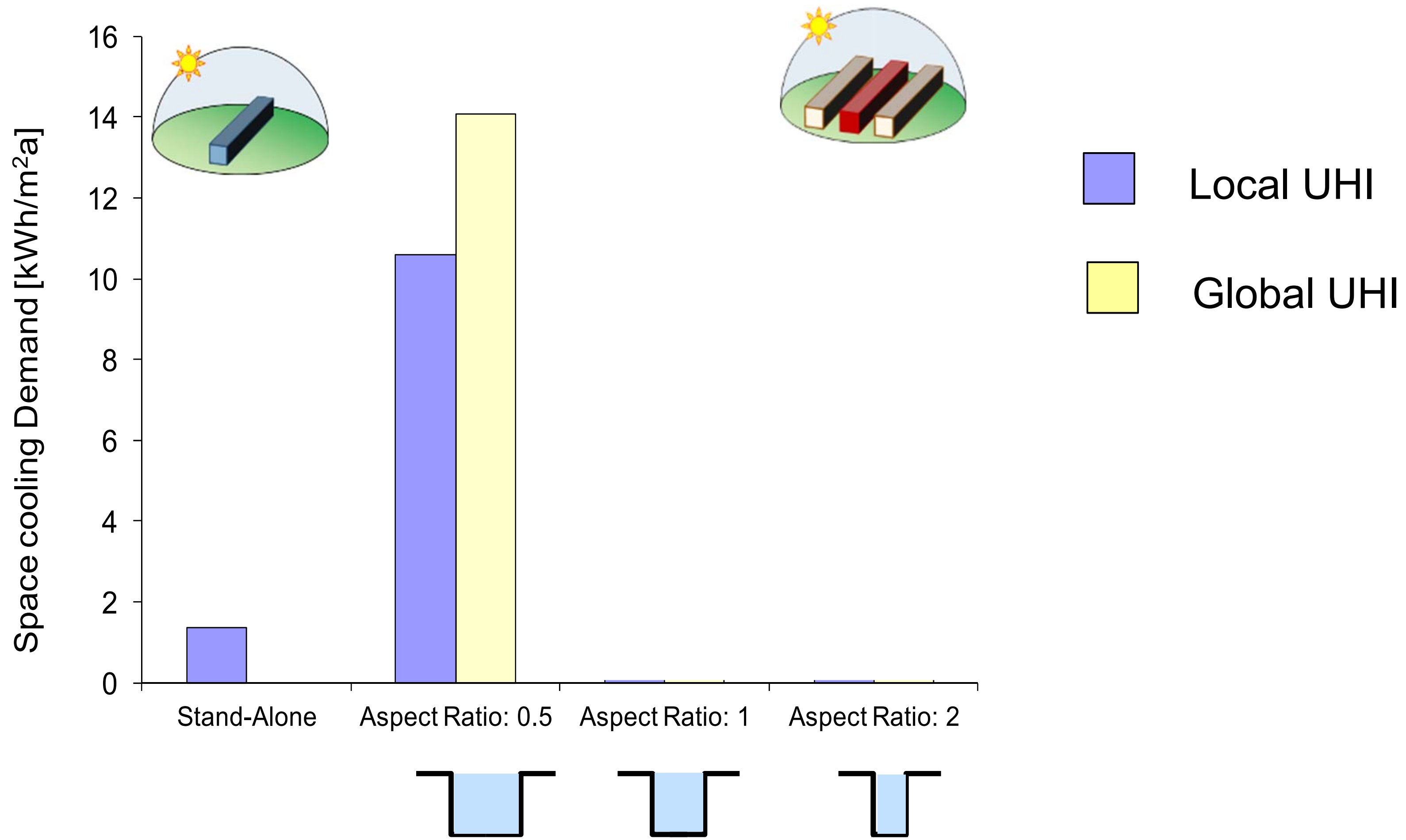
b+c) full coupling

Increase in building cooling demand mainly due to higher air temperatures by local heat islands

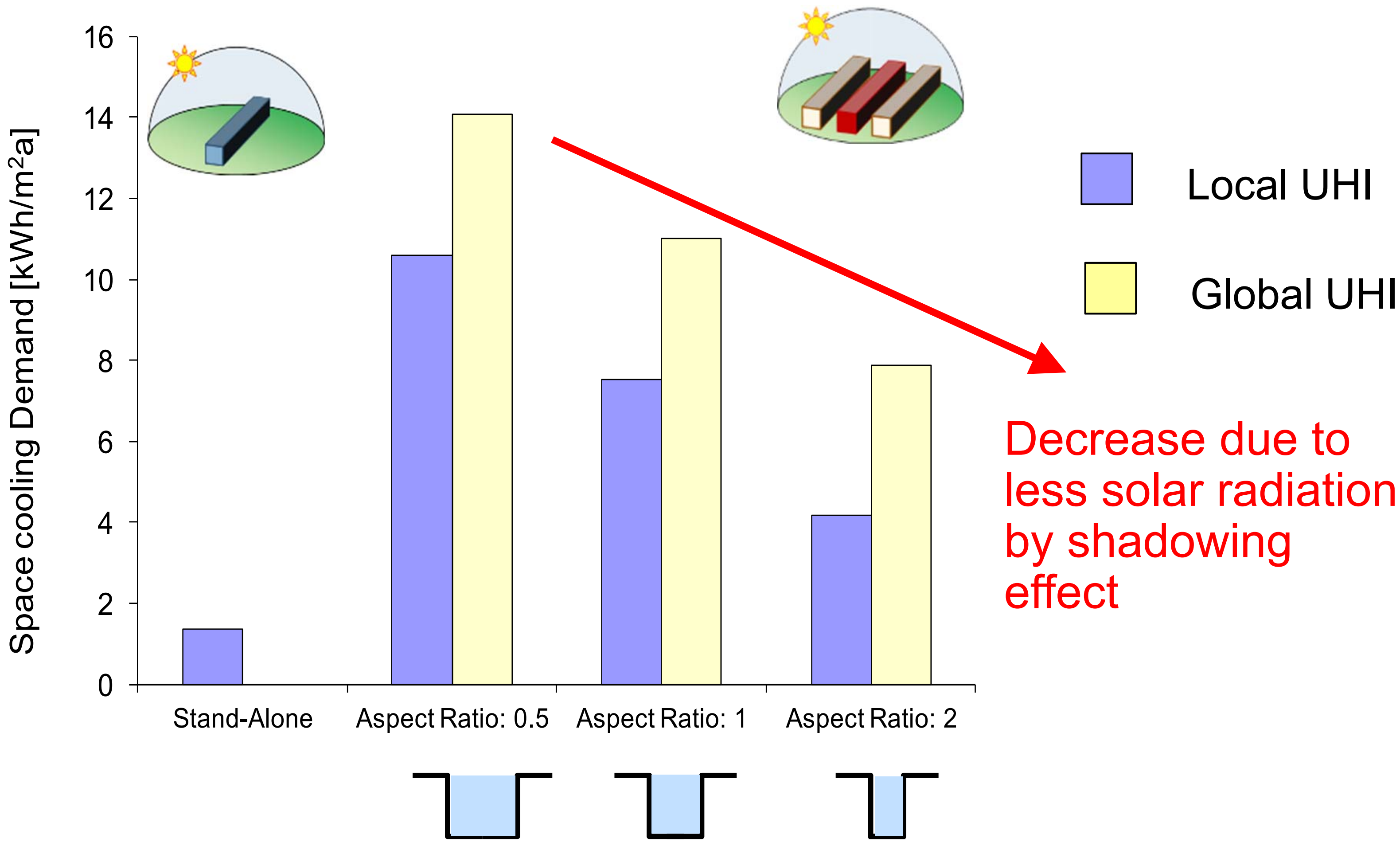
Cooling demands for **local** and **global** urban heat island effect



Cooling demands for **local** and **global** urban heat island effect

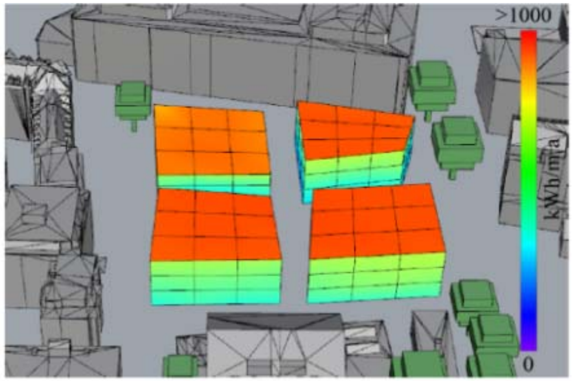


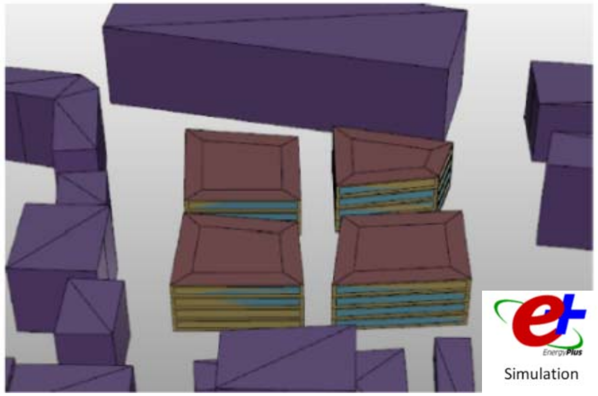
Cooling demands for **local** and **global** urban heat island effect



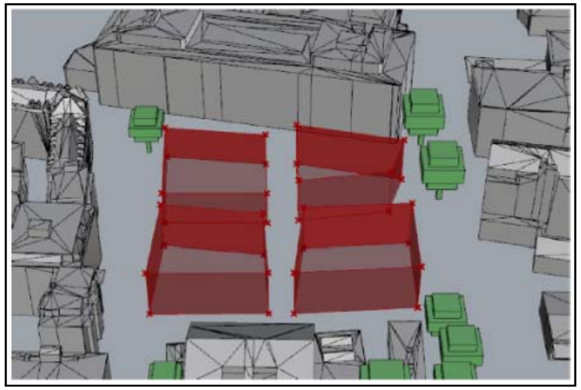
Coupling of urban climate, building energy demand, **building design, building energy system**

Urban climate
Solar potential

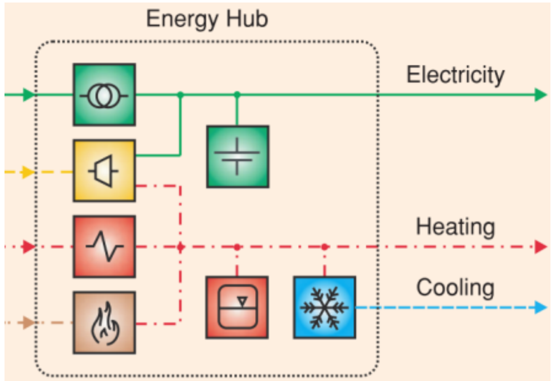




Building energy demand



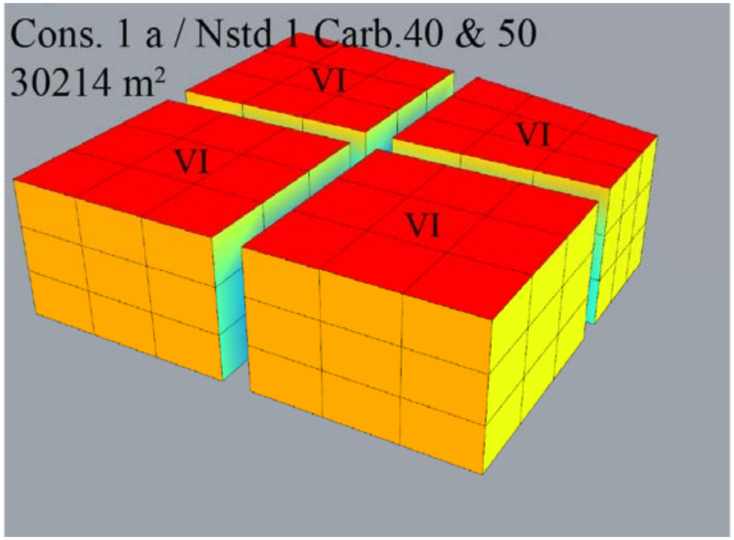
Building design

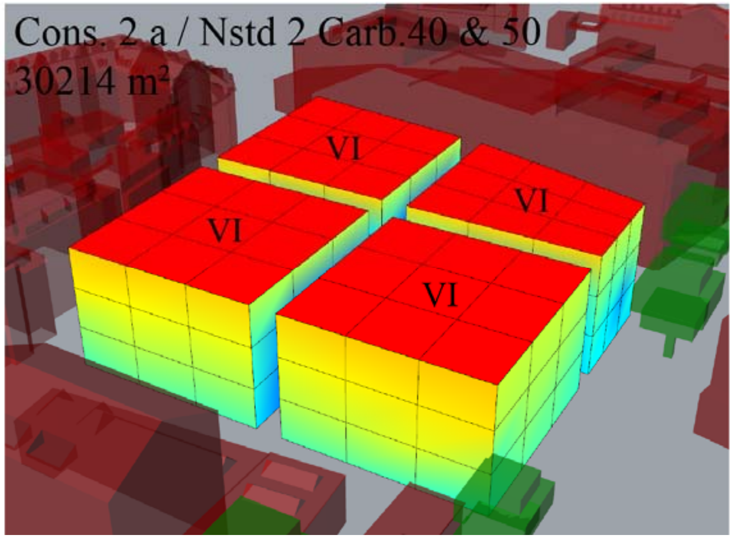


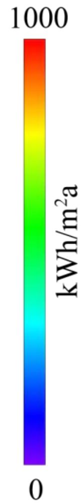
Building systems
Energy Hub

Optimized building forms for different emission constraints

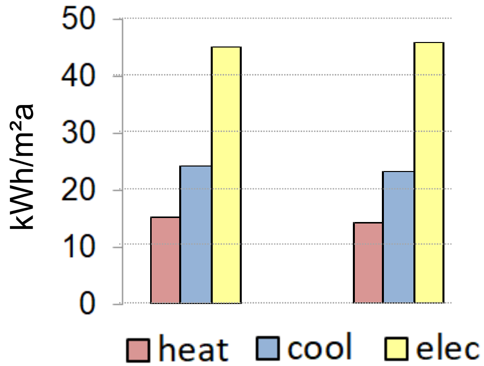
emission constraint: 50 $kgCO_2/m^2a$





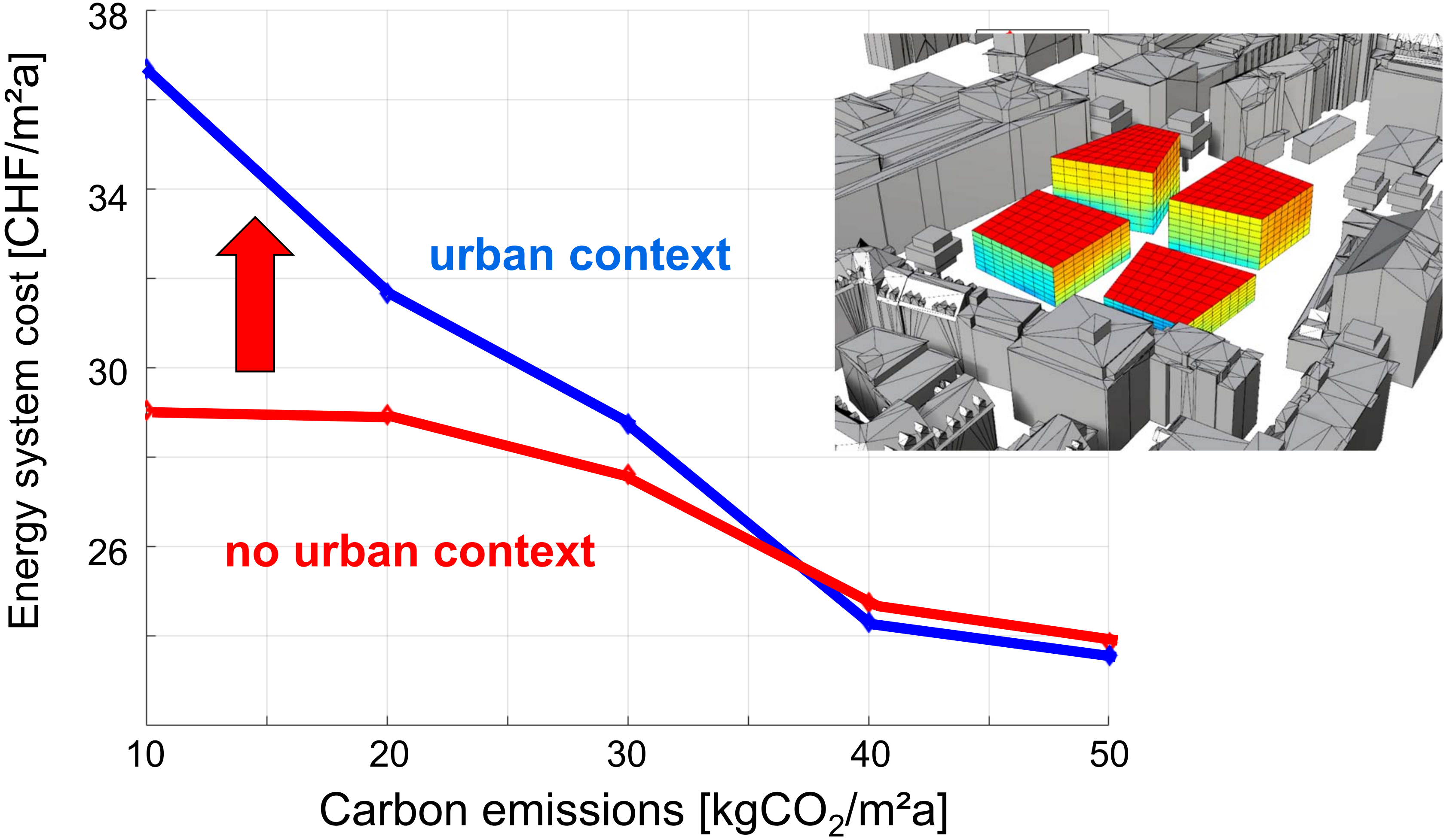


No context



Urban context

Energy system cost and emissions targets through optimization



higher costs in urban context due to less solar potential

Three main actions to reduce cooling demand

- Improvement building energy performance
- Improvement of mechanical air conditioning, alternative cooling technologies
- Mitigation of the global and local climate change

Connected presentations:

Multi-stage optimal design of energy systems for urban districts,
Monday 2:00 PM, George Mavromatidis

Studying the impact of local urban heat islands on the space cooling demand of buildings using coupled CFD and building energy simulations, **Monday 2:30 PM, Jonas Allegrini**

A GIS based methodology to support multi-criteria decision making for the retrofitting process of residential buildings,
Tuesday 11:00 AM, Kristina Orehounig

Questions

What is the impact of urban and local climate under climatic change on

- Urban thermal and wind comfort, heat stress, health (pollutants)
- Building & urban (cooling) energy demand
- **Hygrothermal performance and durability building envelopes**

Observation

Most durability models use **hygrothermal** indicators (temperature, RH) and not (direct) **damage** related indicators

Questions

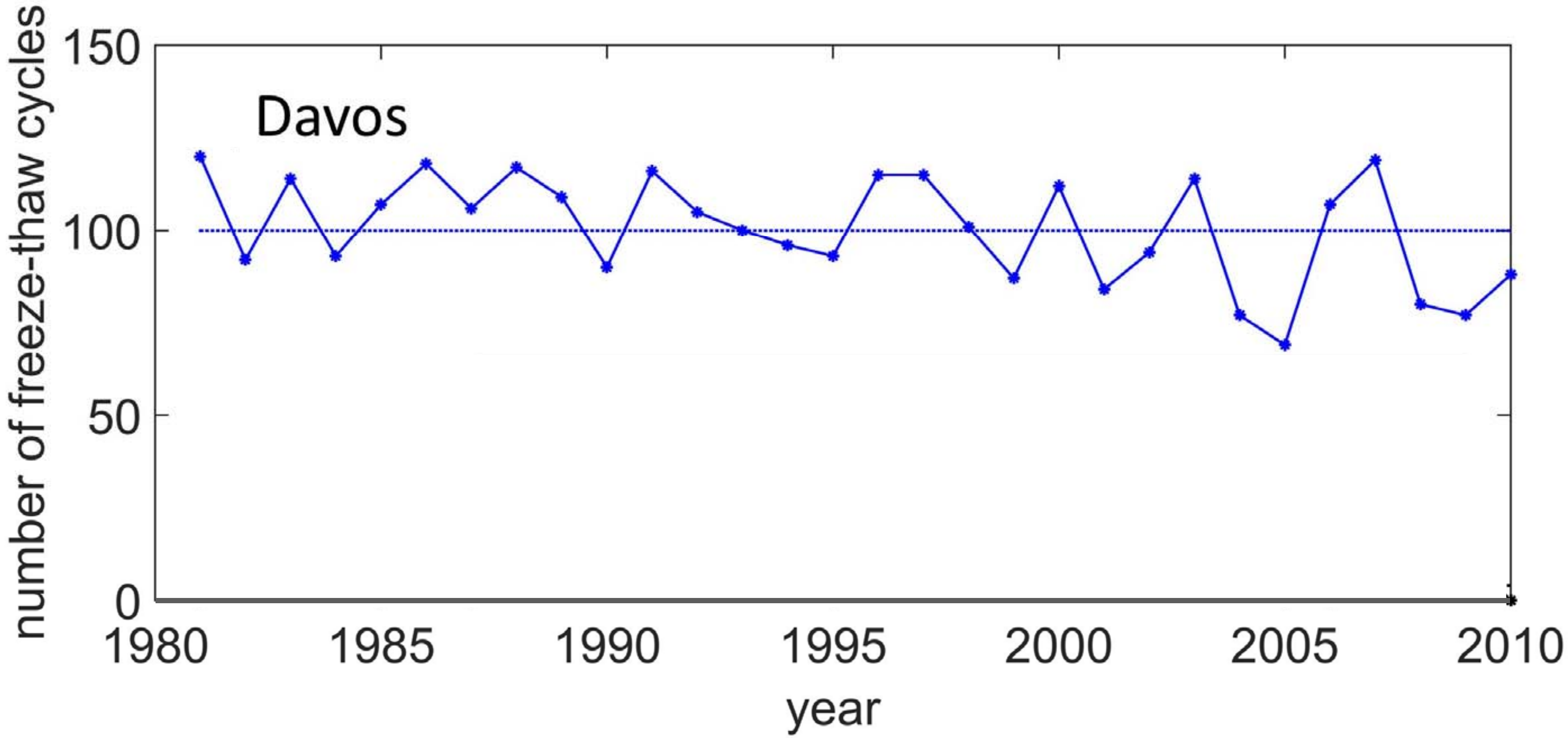
- Which durability methodology ?
- Will the risk for moisture related damage in(de)crease due to climate change ?

Challenge

- development of adequate moisture durability models
- Example: frost damage model

Classical approach: hygrothermal analysis (no freezing modelling)

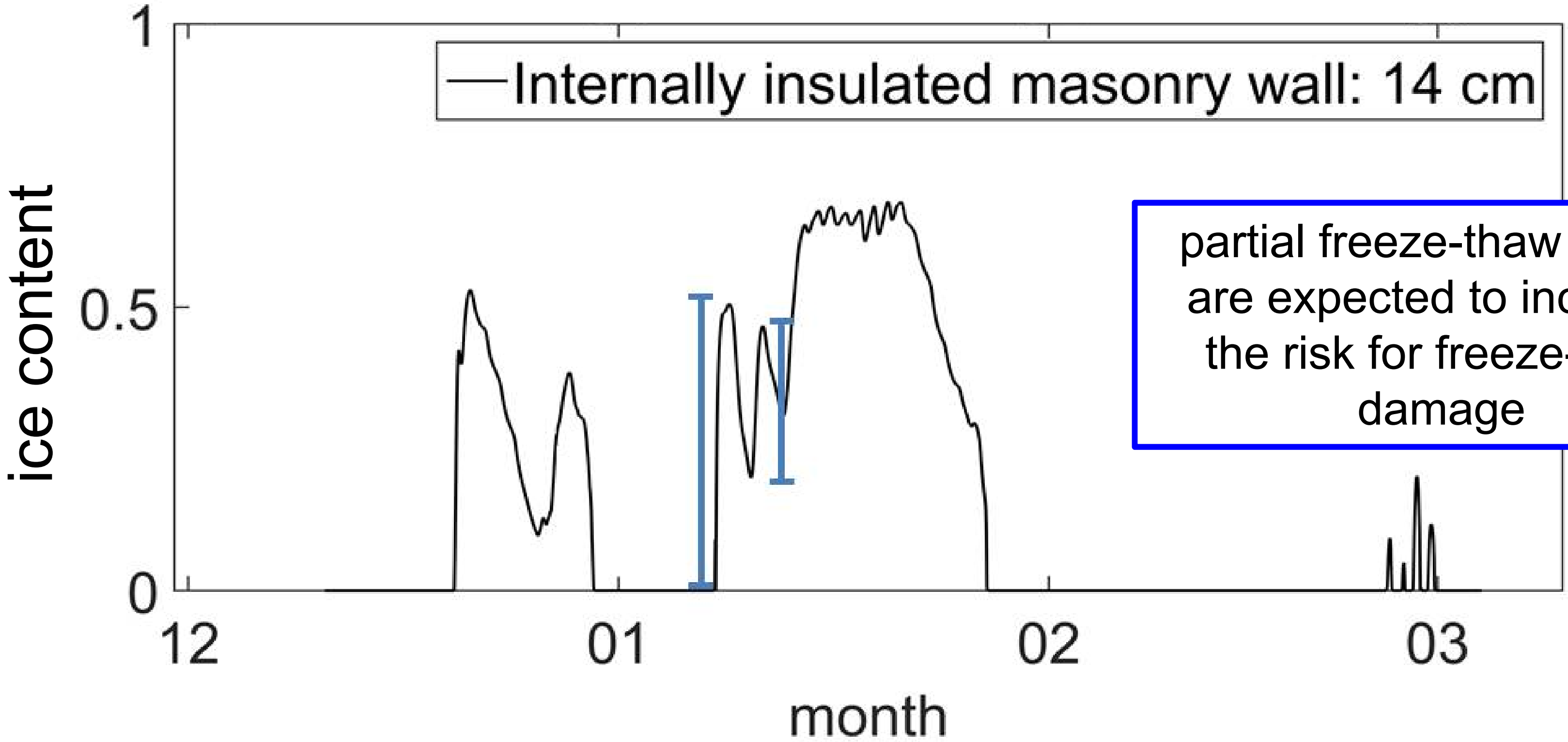
Number of freeze / thaw cycles based on temperature crossing at zero degrees



New approach: hygrothermal analysis including freezing modelling

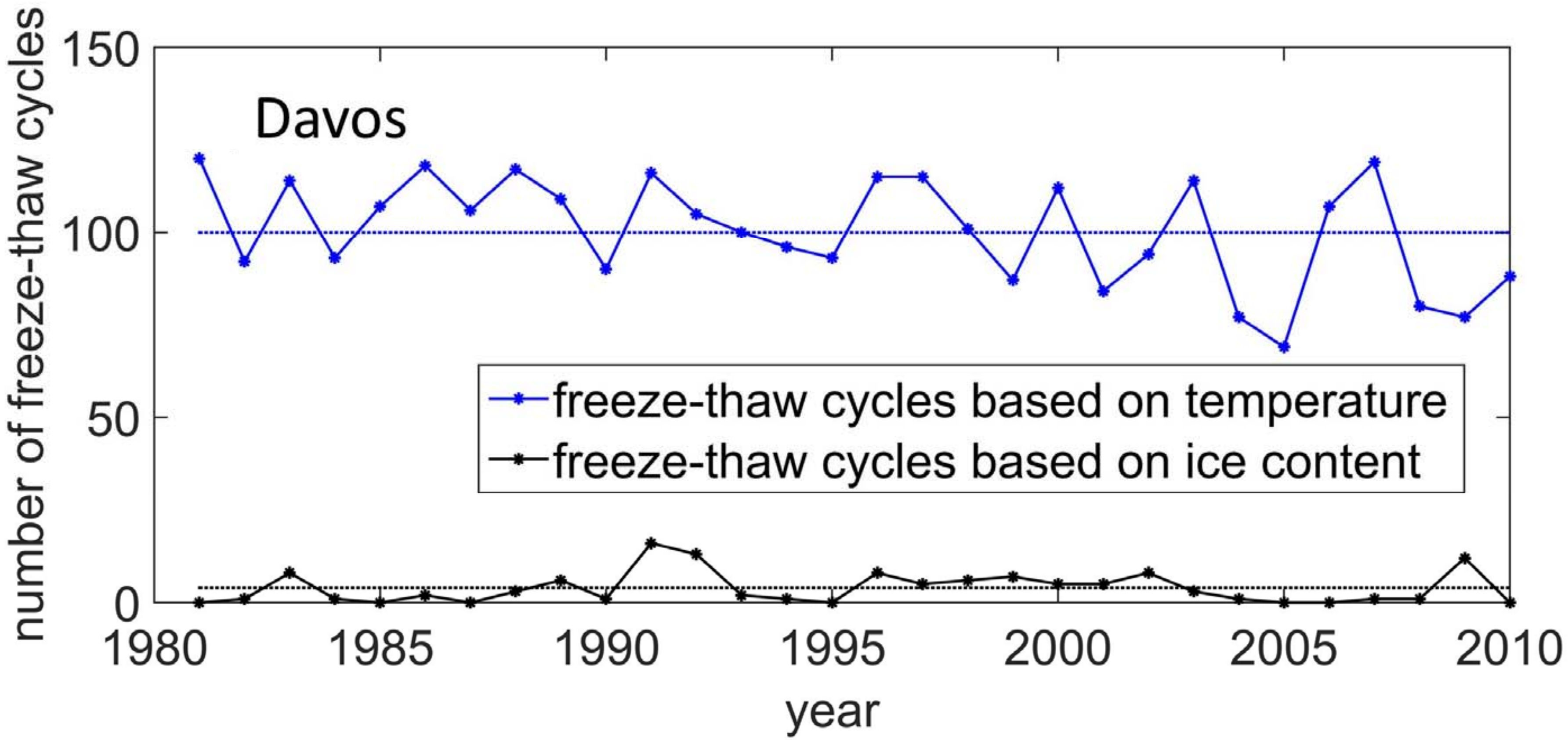
New damage risk index based on changes in ice content

Freeze-thaw damage risk index $= \sum_{cycle} (S_{\text{ice,max}} - S_{\text{ice,min}})$



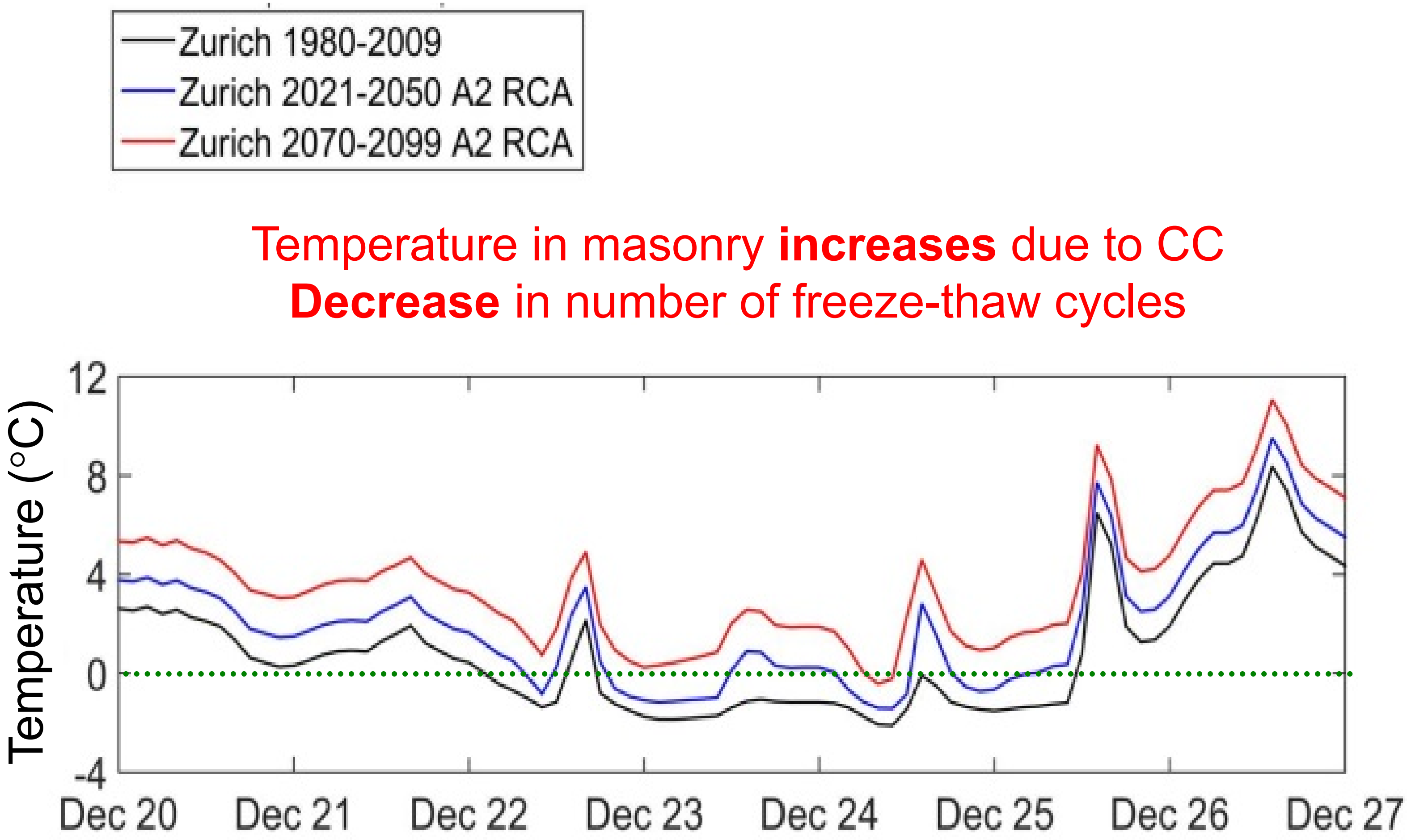
partial freeze-thaw cycles are expected to increase the risk for freeze-thaw damage

Comparison two approaches



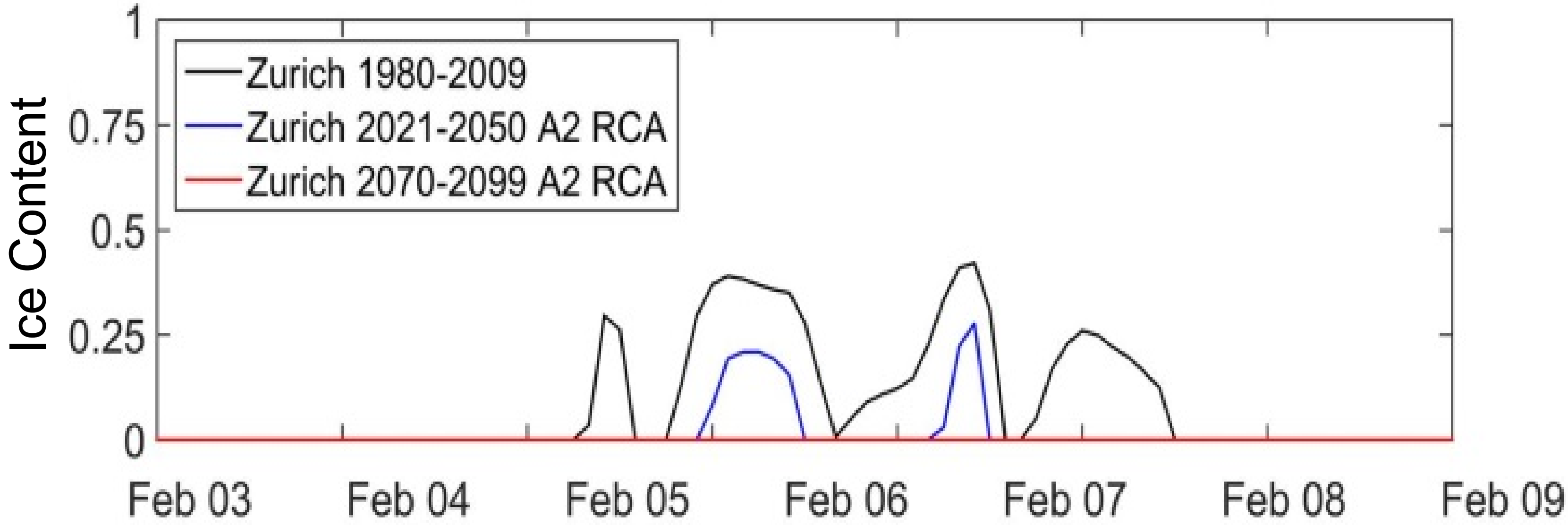
Influence of climate change on frost damage masonry with inside insulation

Zurich



Influence of climate change on frost damage masonry with inside insulation

Zurich

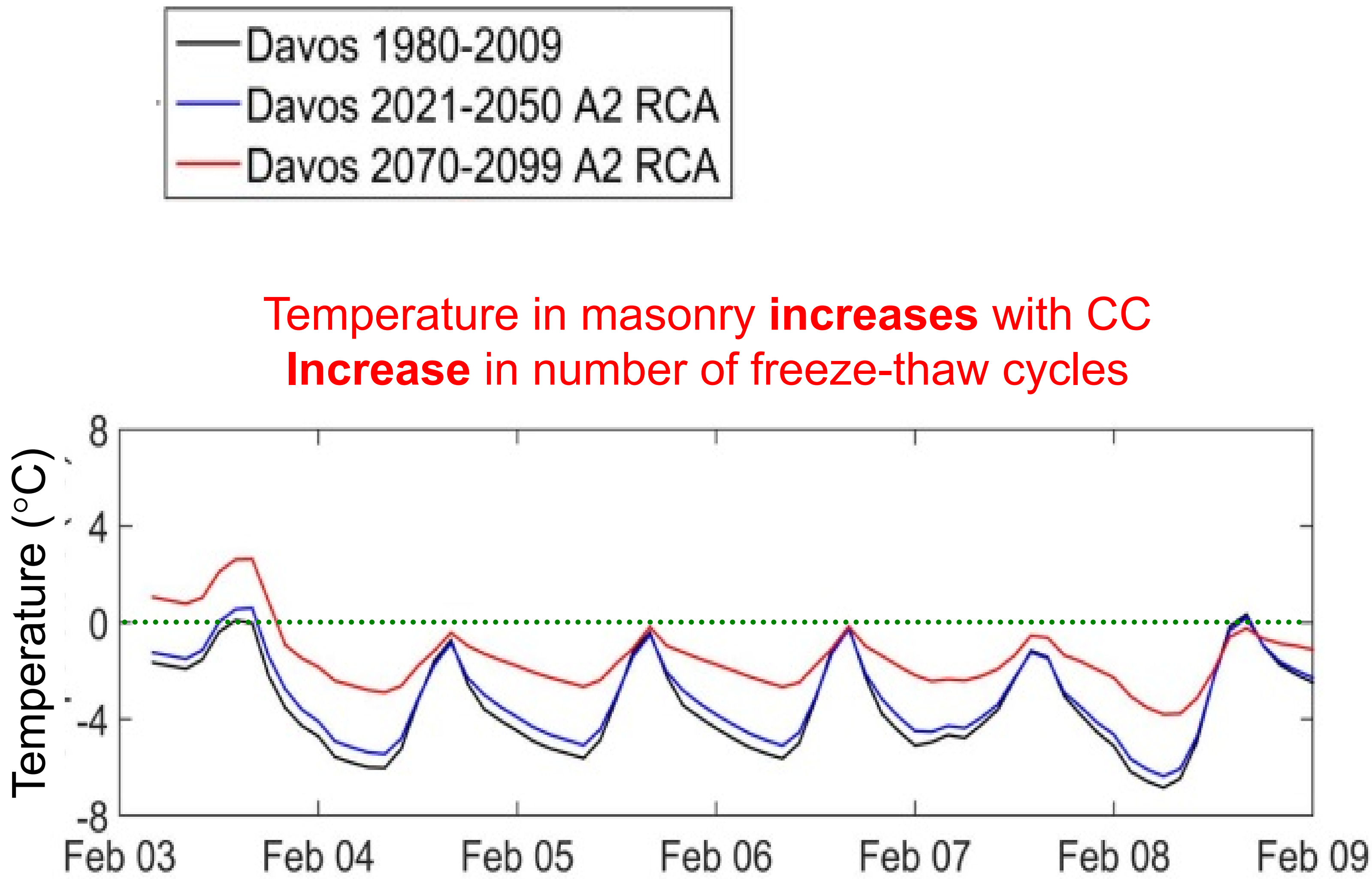


Ice content in masonry **decreases** with CC
Decrease in number of freeze-thaw cycles
no freezing by 2070

Less damage expected with CC

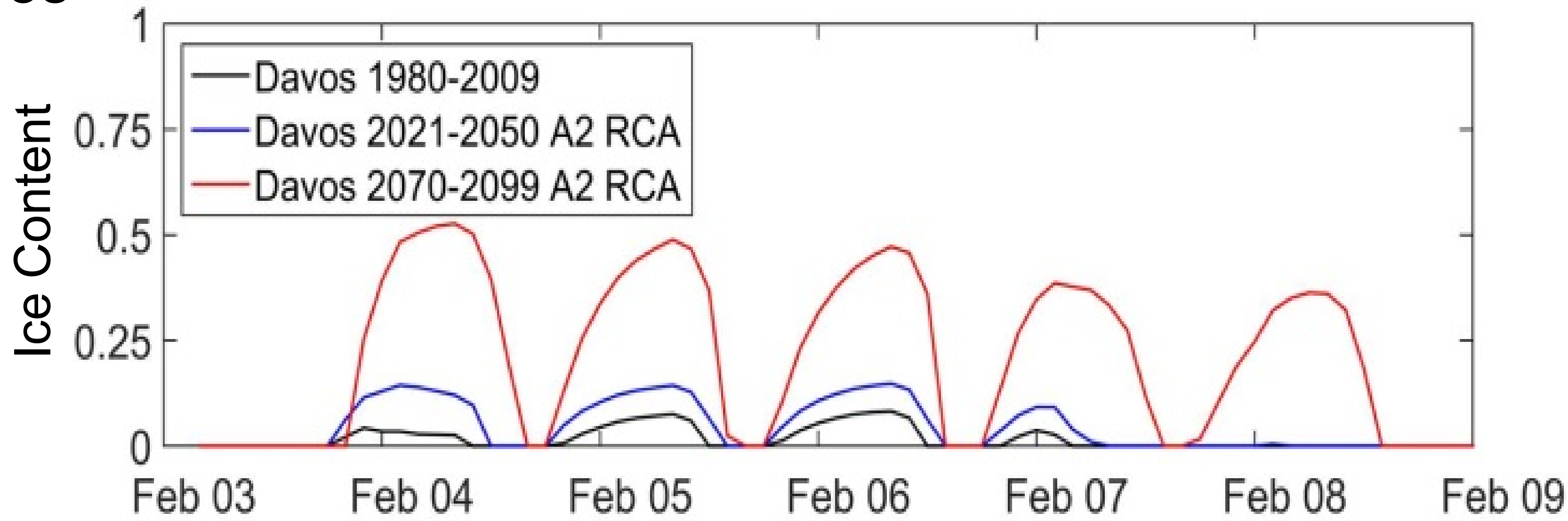
Influence of climate change on frost damage masonry with inside insulation

Davos



Influence of climate change on frost damage masonry with inside insulation

Davos



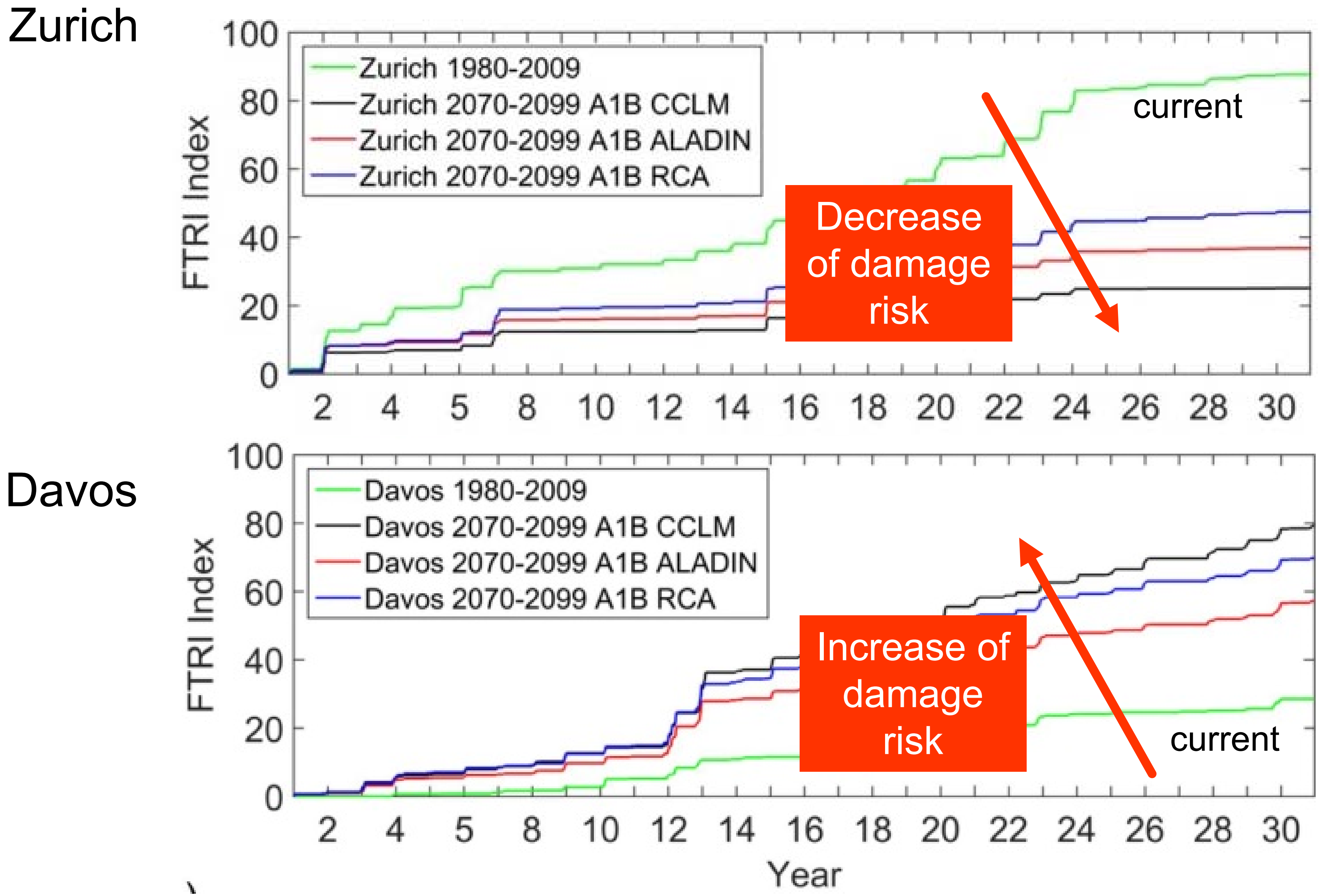
Ice content in masonry **increases** with CC

Increase in number of freeze-thaw cycles

Snow becomes rain: increase in moisture content

More damage expected with CC

Cumulative frost damage index for next 30 years



Connected presentations:

Water uptake in masonry: effect of brick/mortar interface,
Monday 11:00 AM , **Xiaohai Zhou**

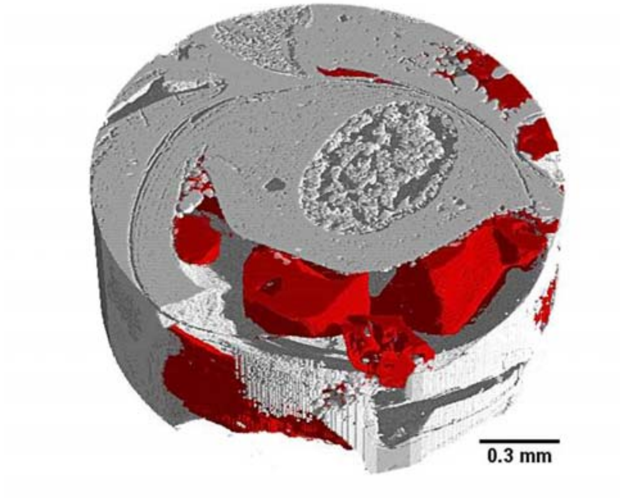
Adsorption and film forming of train of water droplets impacting porous stones, **Monday 11:45 AM,** **Dominique Derome**

Open challenges for improved heat-air-mass transfer analysis including phase change

- Multiscale experiments from pore to macroscale

Example of crystallization damage

Bi-pyramidal structure of heptahydrate crystal in macropores

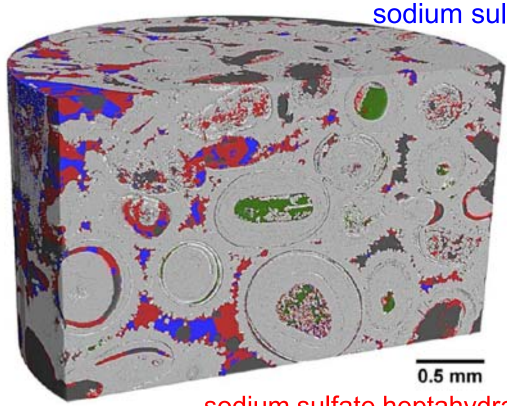


PhD H. Derluyn 2012

Crystal growth in pore space

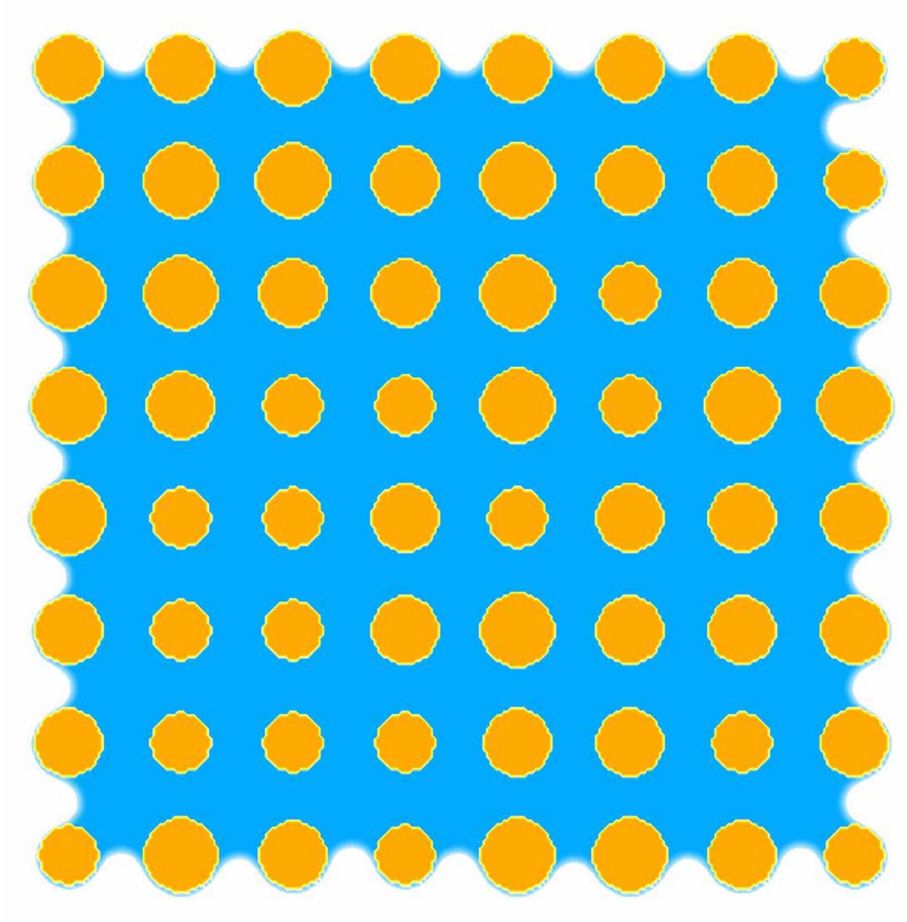
Phases in drying salt solution

Cooling of 2.8m Na_2SO_4 solution to -6 °C



Open challenges for improved heat-air-mass transfer analysis including **phase change**

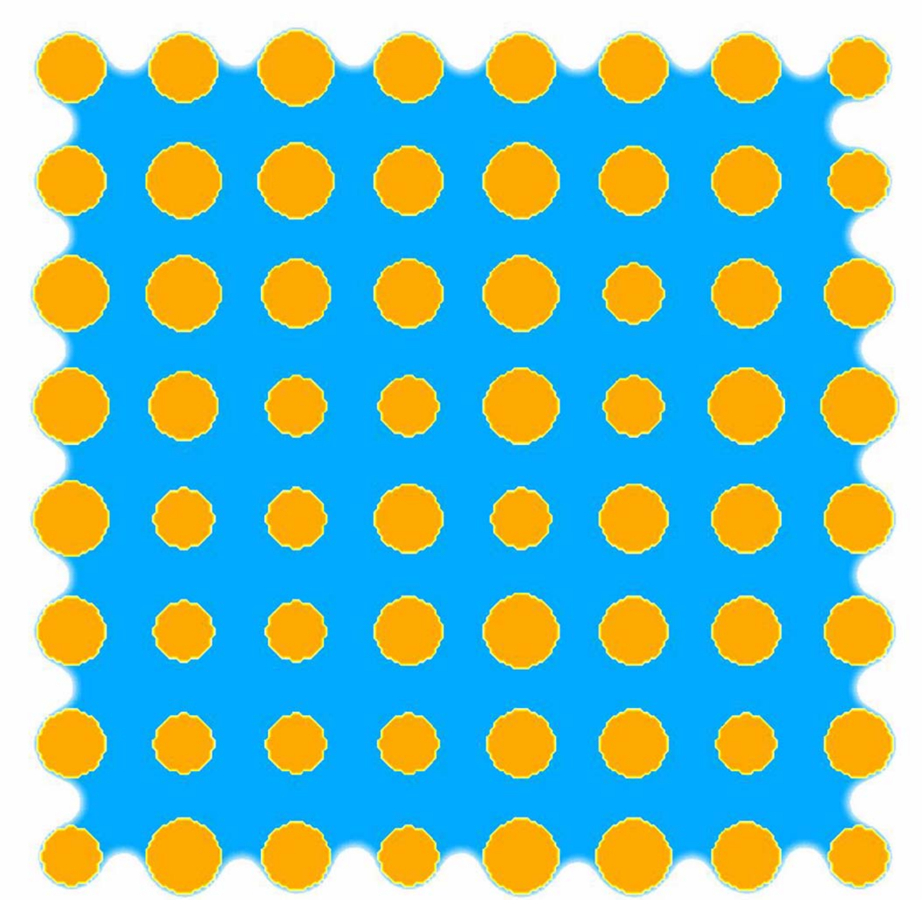
- Modelling at pore scale by lattice Bolzmann modelling



Drying of water in porous medium without salts

Open challenges for improved heat-air-mass transfer analysis including **phase change**

- Modelling at pore scale by lattice Bolzmann modelling

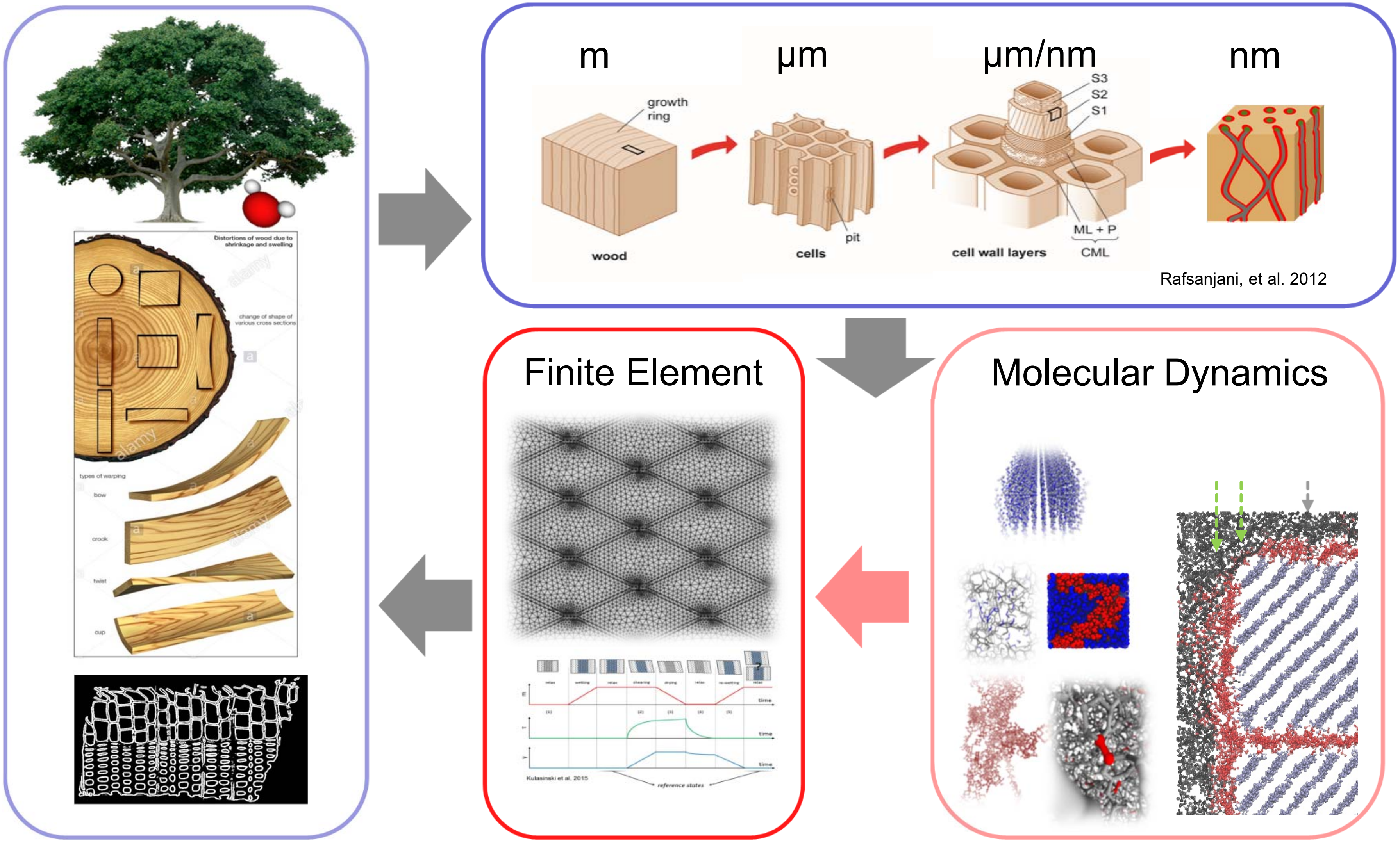


Salt bridges form over pores blocking the drying of the solution

Drying of water in porous medium with salts

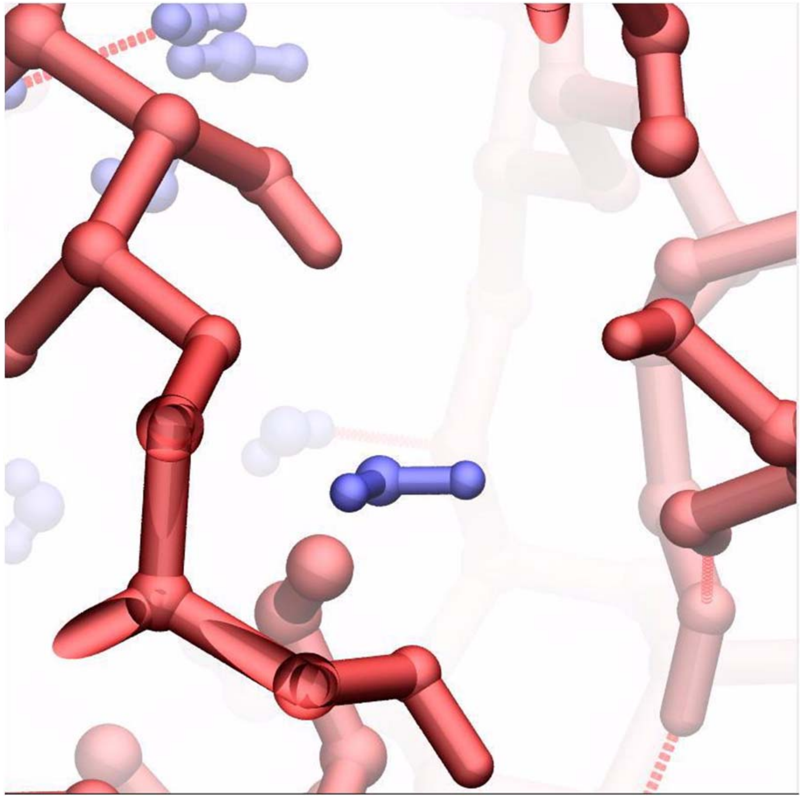
Open challenges for improved heat-air-mass transfer analysis including phase change and **mechanics**

- Multiscale approach for wood

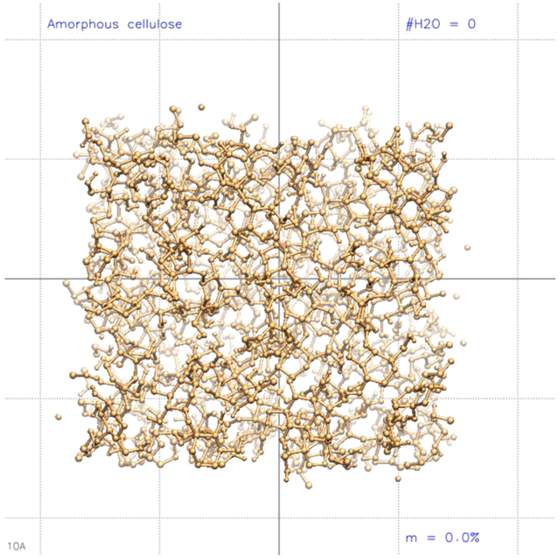


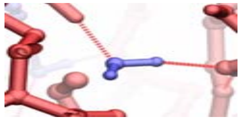
Example: sorption and swelling in wood

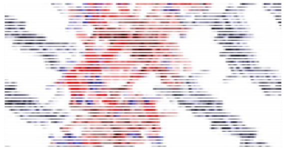
- Nanoscale: wood, molecular dynamics



Sorption and swelling

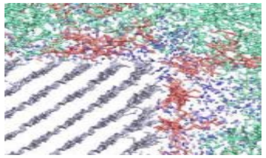




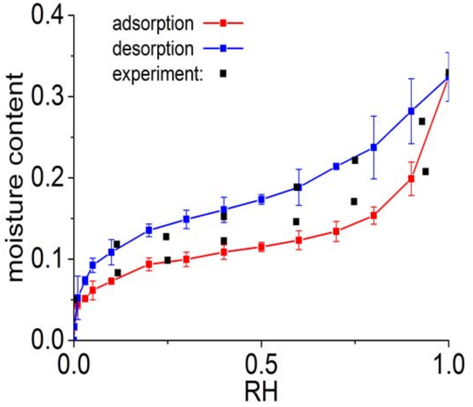


crystalline cellulose

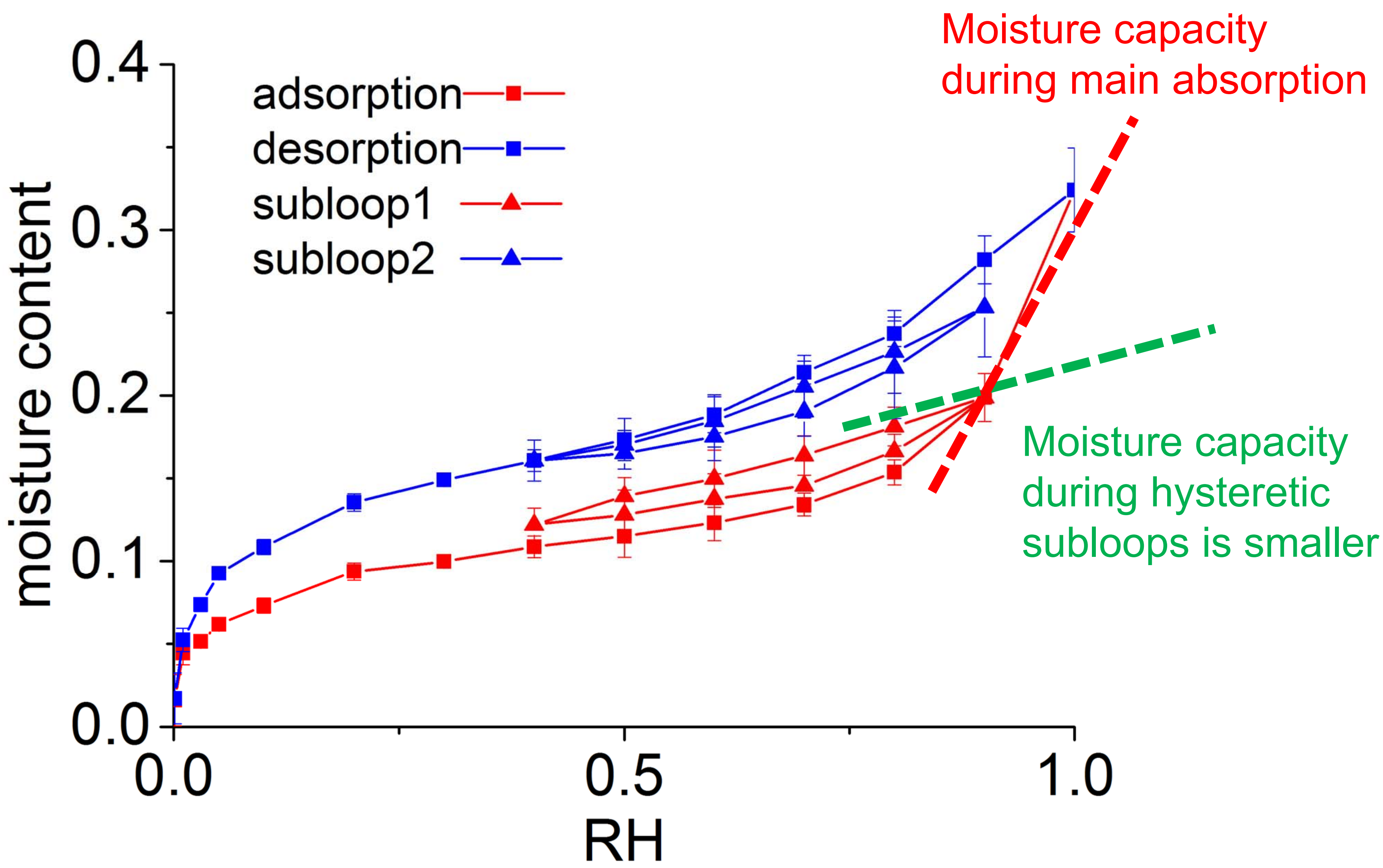
lignin



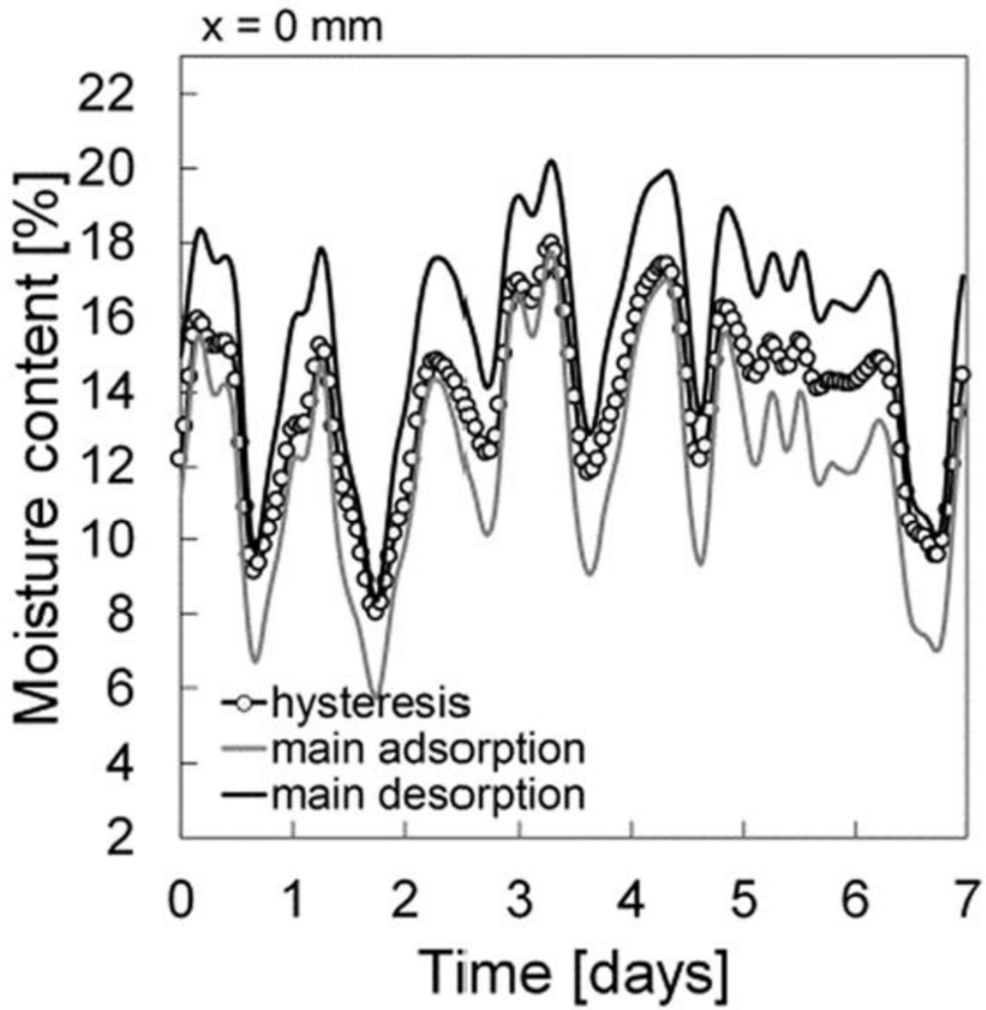
sorption hysteresis:
modelling and experiment



Hysteresis during sorption

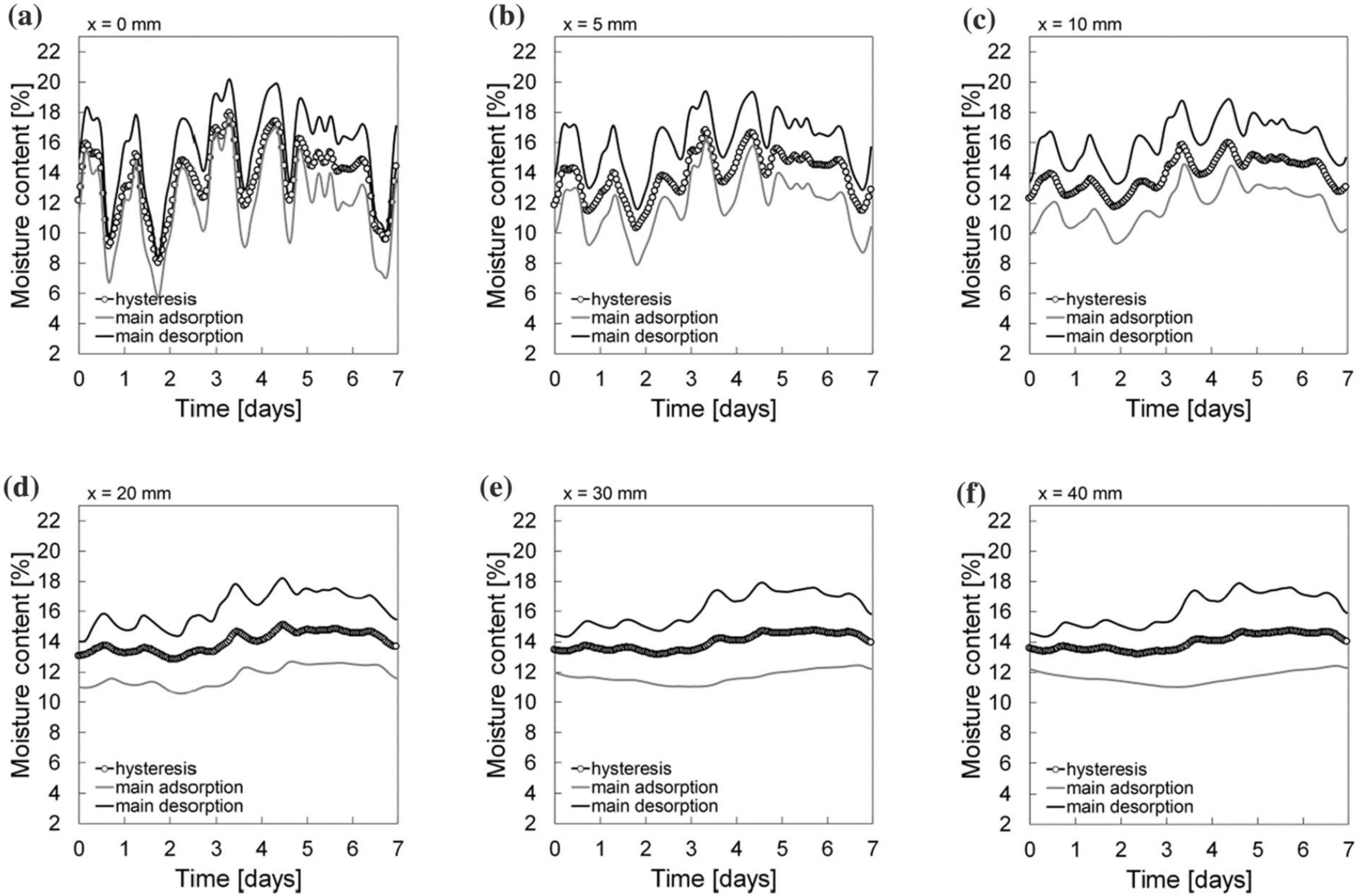


Moisture content variations in wooden specimen exposed to climatic fluctuations



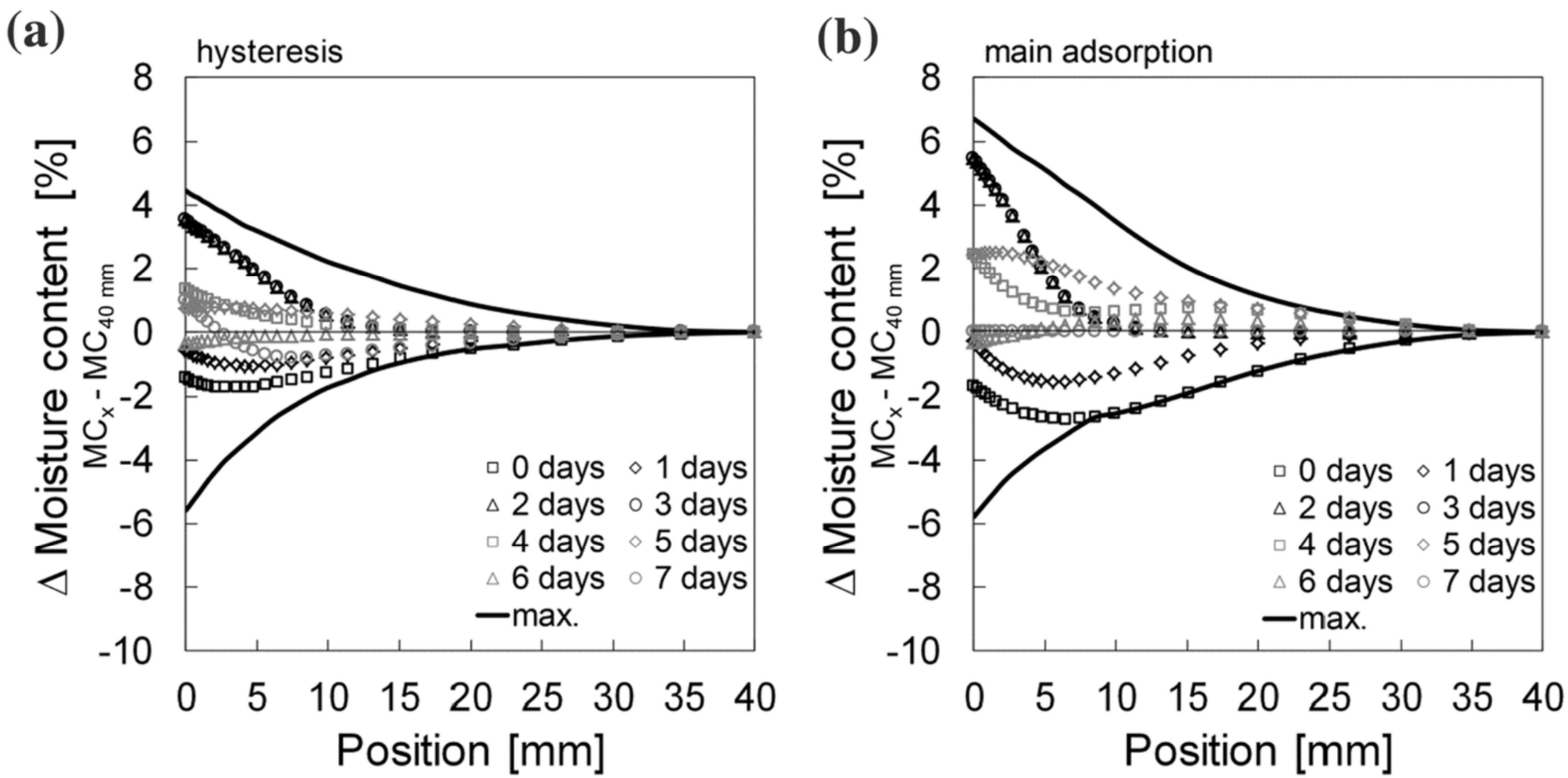
Moisture variations smaller in hysteresis than in main ad- and desorption

Moisture content variations in wooden specimen



Moisture variations smaller deeper in the material

Moisture content variations in wooden specimen



Hysteresis **Main adsorption**

Moisture variations smaller in hysteresis than in main adsorption

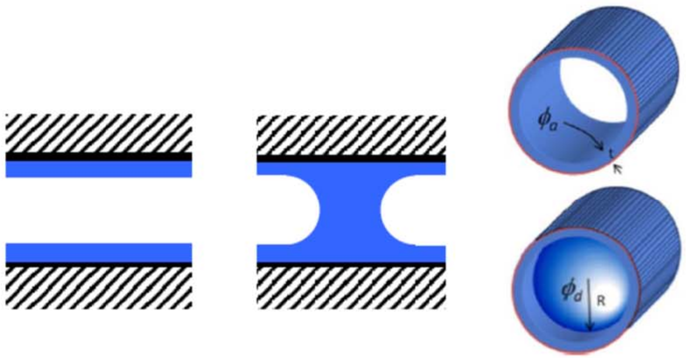
Origin of hysteresis

in macroporous capillary active materials

Capillary condensation hysteresis

Origin of sorption hysteresis

Capillary condensation



$$RT \ln \frac{P_A}{P_0} = -\frac{\gamma V_L}{r_p - t_A}$$

$$RT \ln \frac{P_D}{P_0} = -\frac{2\gamma V_L}{r_p - t_D}$$

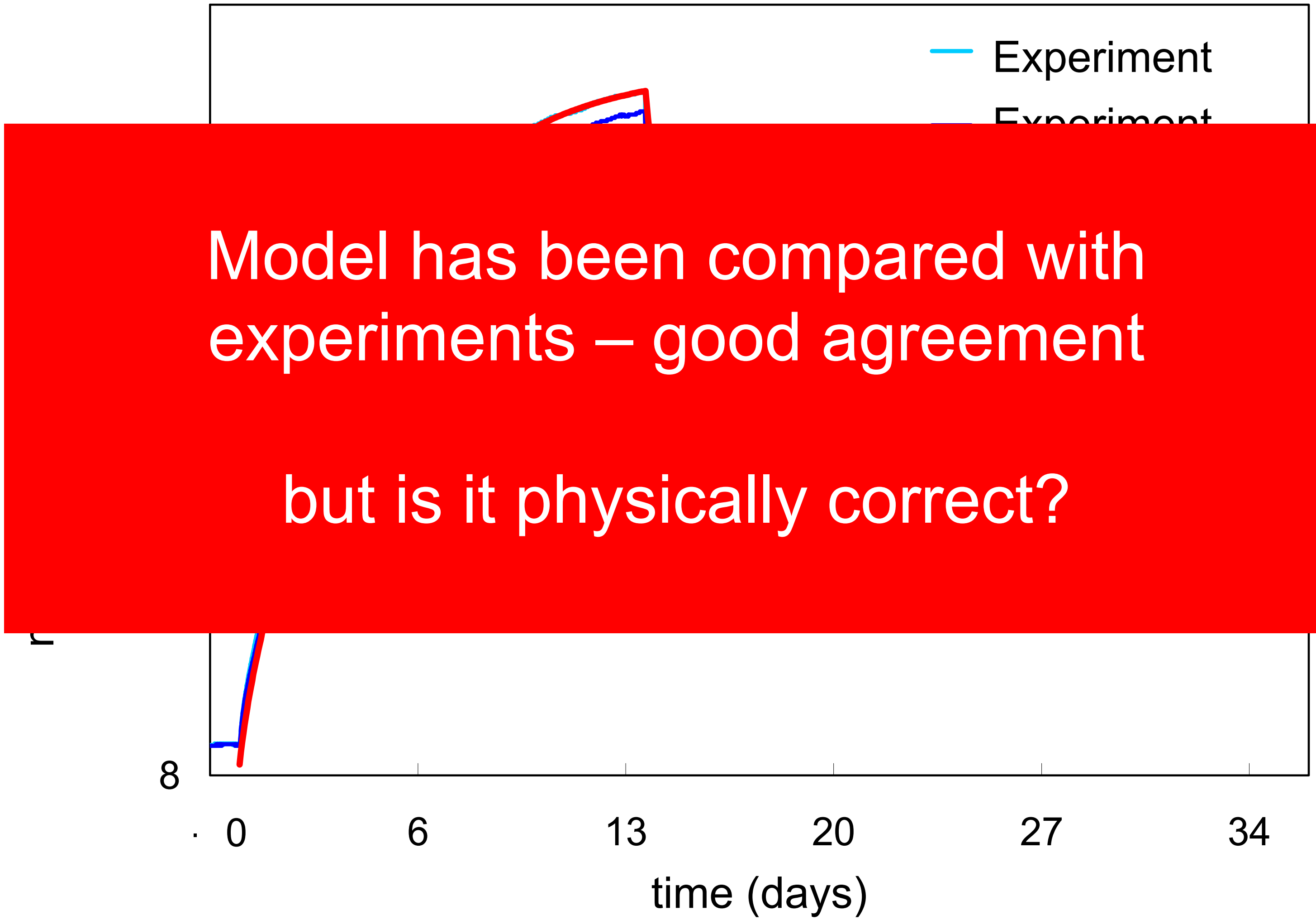
Bottle neck effect


Throat - pore

Inkt bottle pores do not fill and unfill at the same capillary pressure depending on pore throat diameter

Validation: adsorption and desorption loop

Wood (spruce) tangential direction



Model has been compared with experiments – good agreement

but is it physically correct?

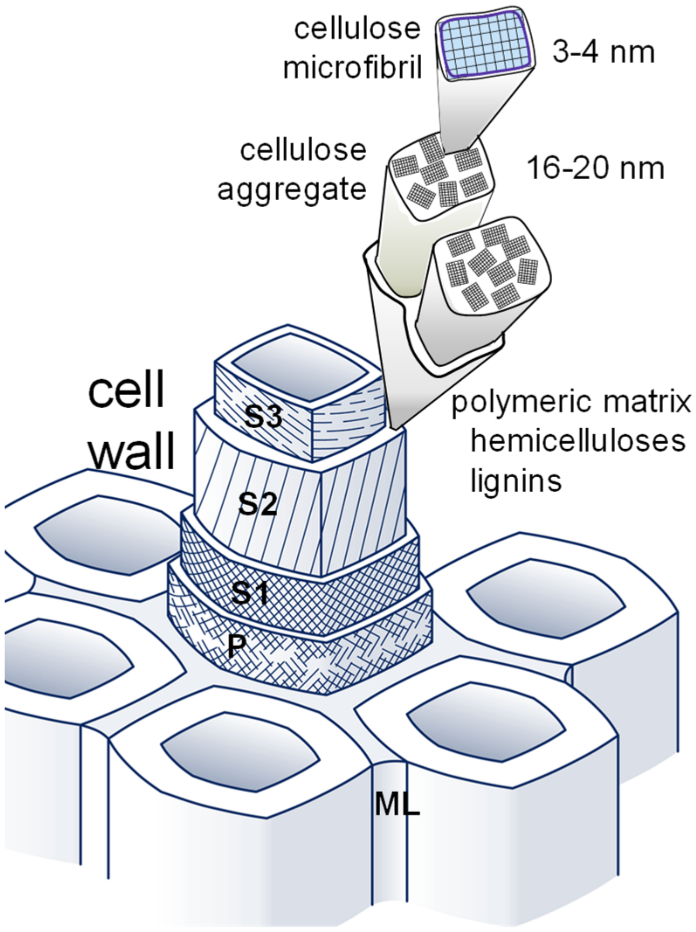
Patera A, Derluyn H, Derome D, Carmeliet J. (2016) Influence of sorption hysteresis on moisture transport in wood. Wood Sc. and Techn. 50:259-283.

Discussion

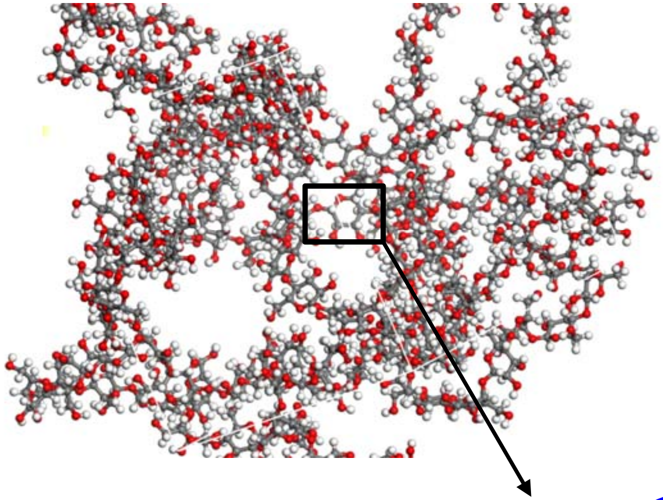
Hysteretic model based on capillary condensation

Applicable to hierarchical nano- porous material such as wood ?

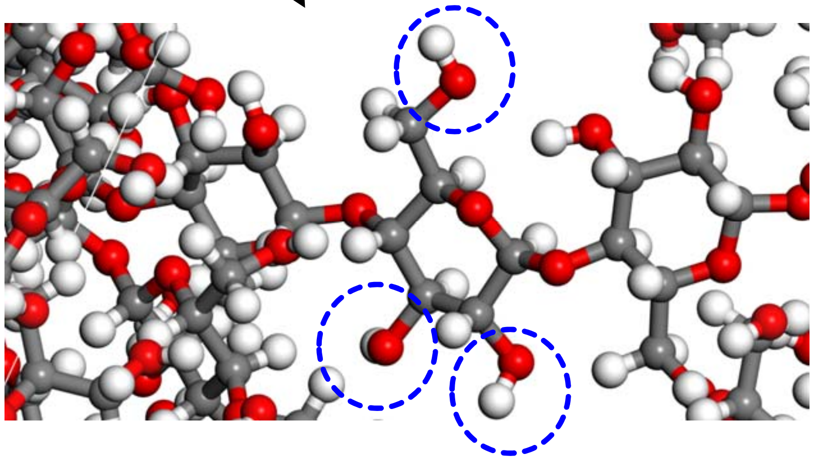
Structure of wood



Atomistic analysis: Sorption hysteresis of amorphous cellulose



3 sorption
sites per ring



O2, O3, and O6
oxygen atoms can form
hydrogen bonds with water

Hydrophilic, porous
1D chains

Kulasinski *et al.*, *Cellulose*, 2014
Kulasinski *et al.*, *ACS Macroletters*, 2014

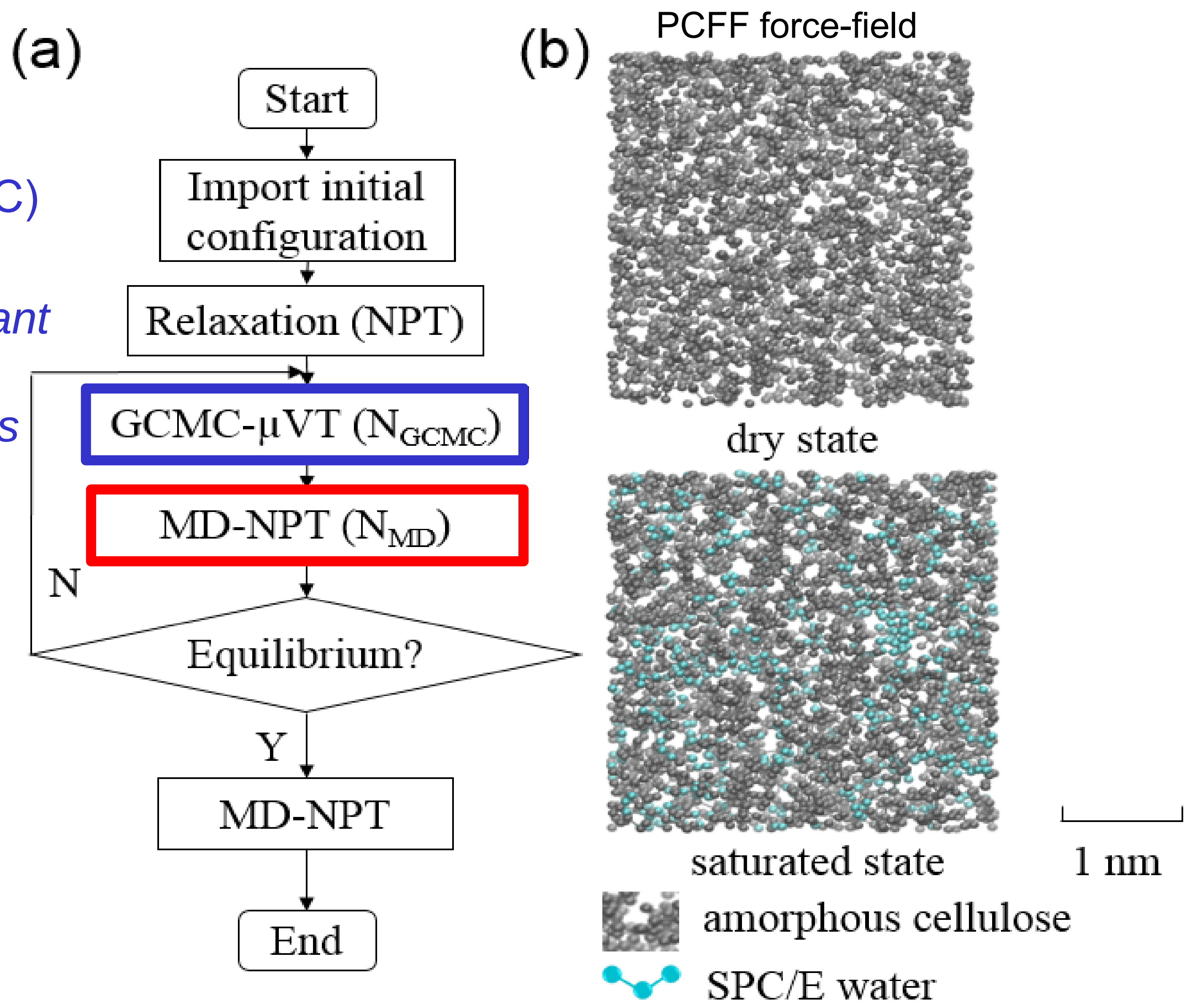
Atomistic simulation of cellulose

Grand canonical Monte Carlo (GCMC)

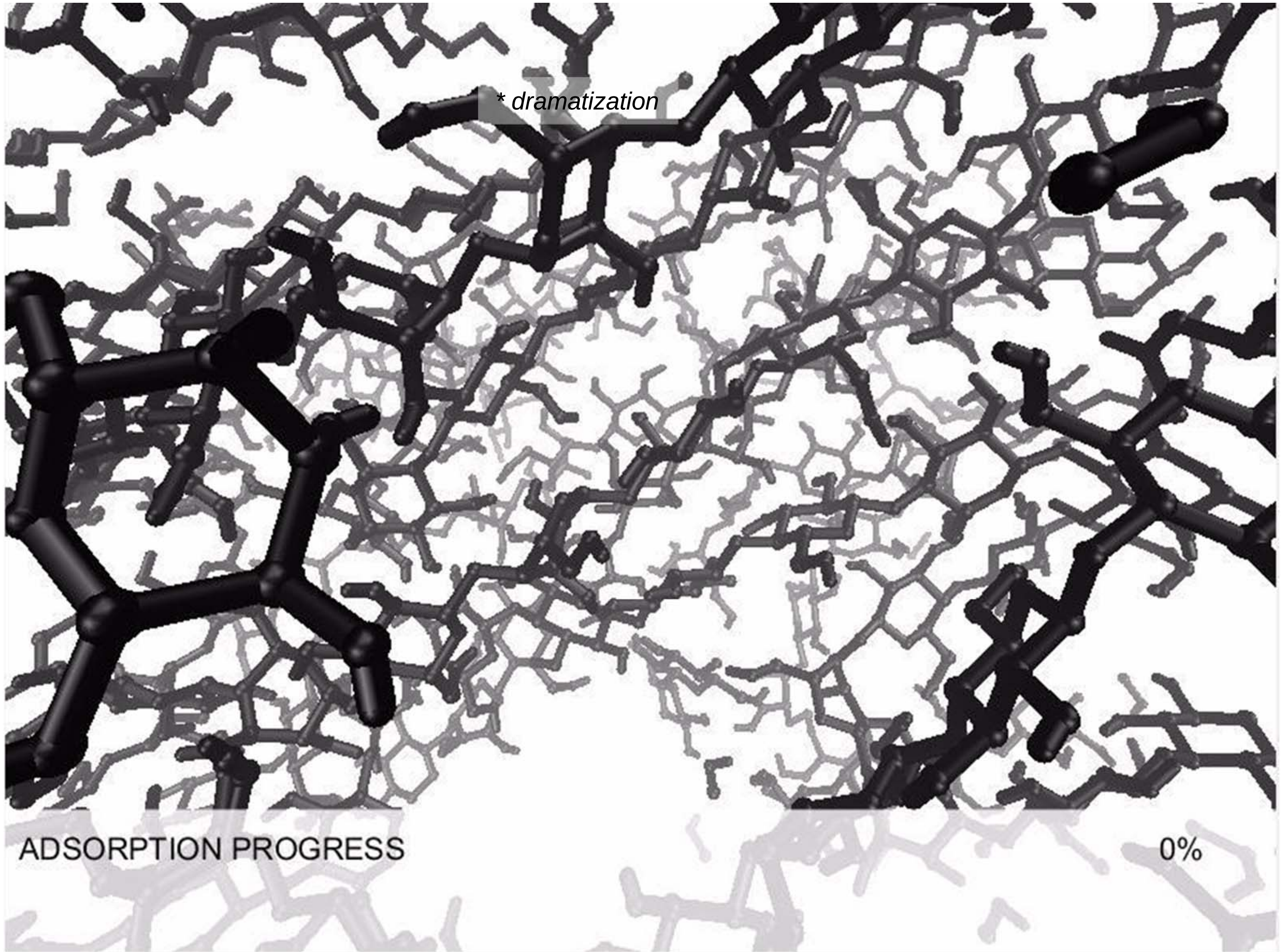
Sorption: insertion molecules at constant volume (V) until chemical potential is reached

Molecular Dynamics (MD)

allowing deformation at constant number of molecules (N)

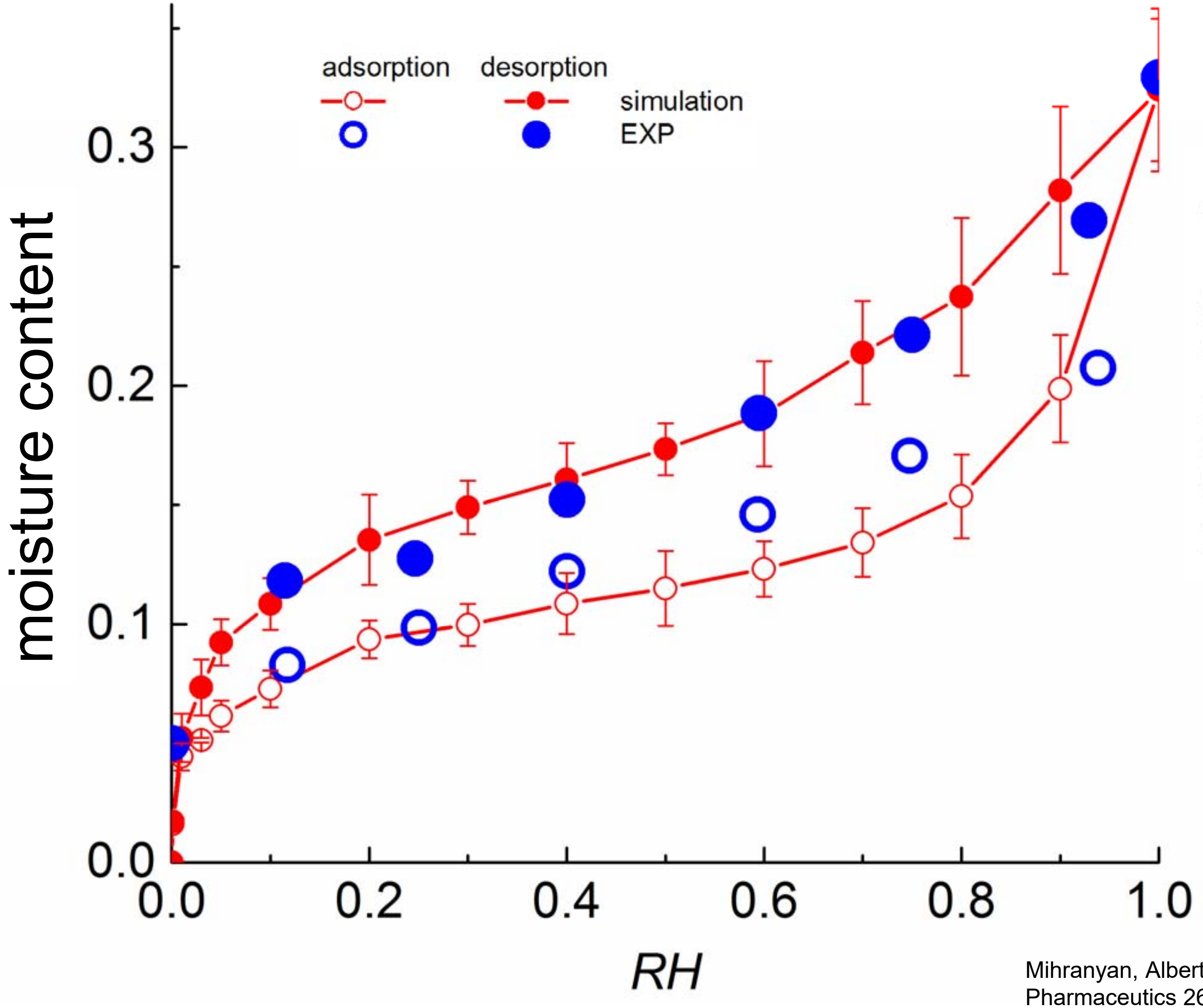


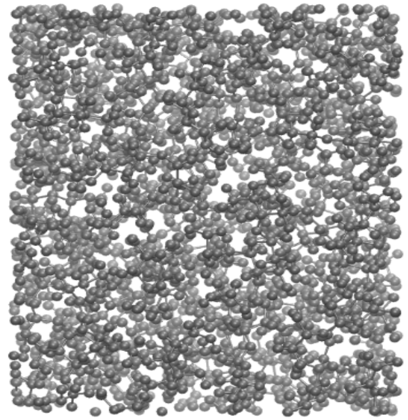
adsorption



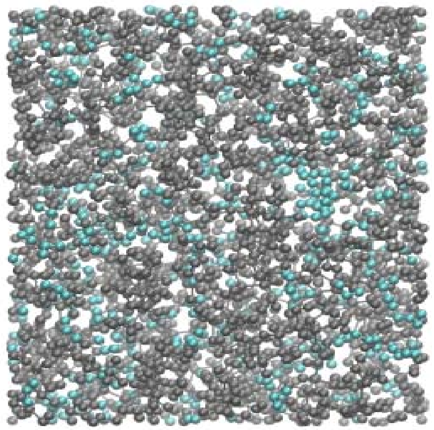
Atomistic simulation

Sorption isotherms





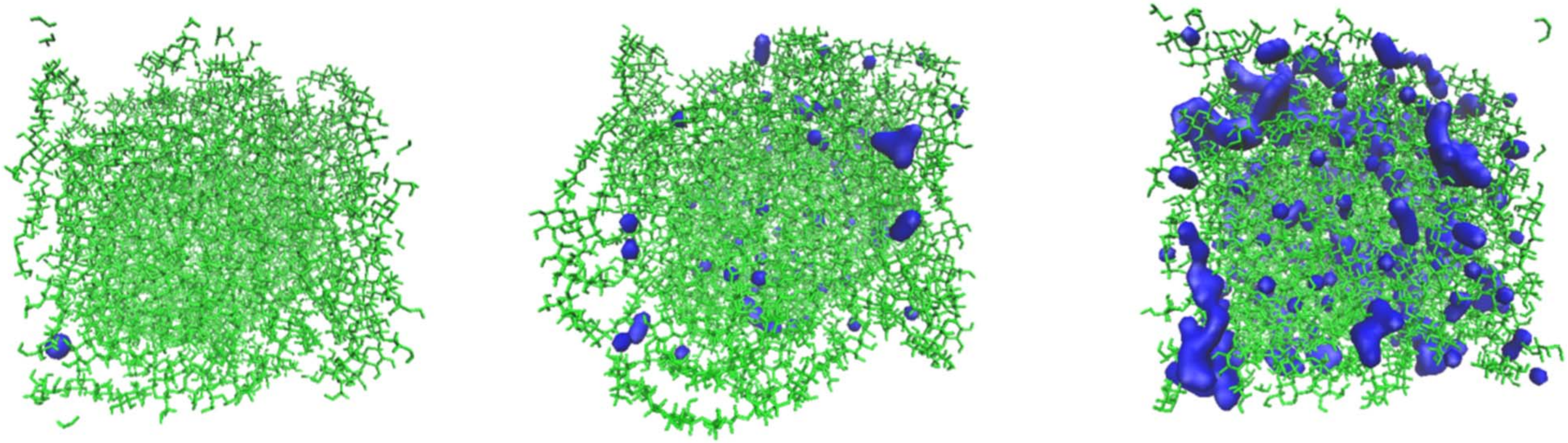
dry state



saturated state

Mihranyan, Albert, et al. International Journal of Pharmaceutics 269.2 (2004): 433-442

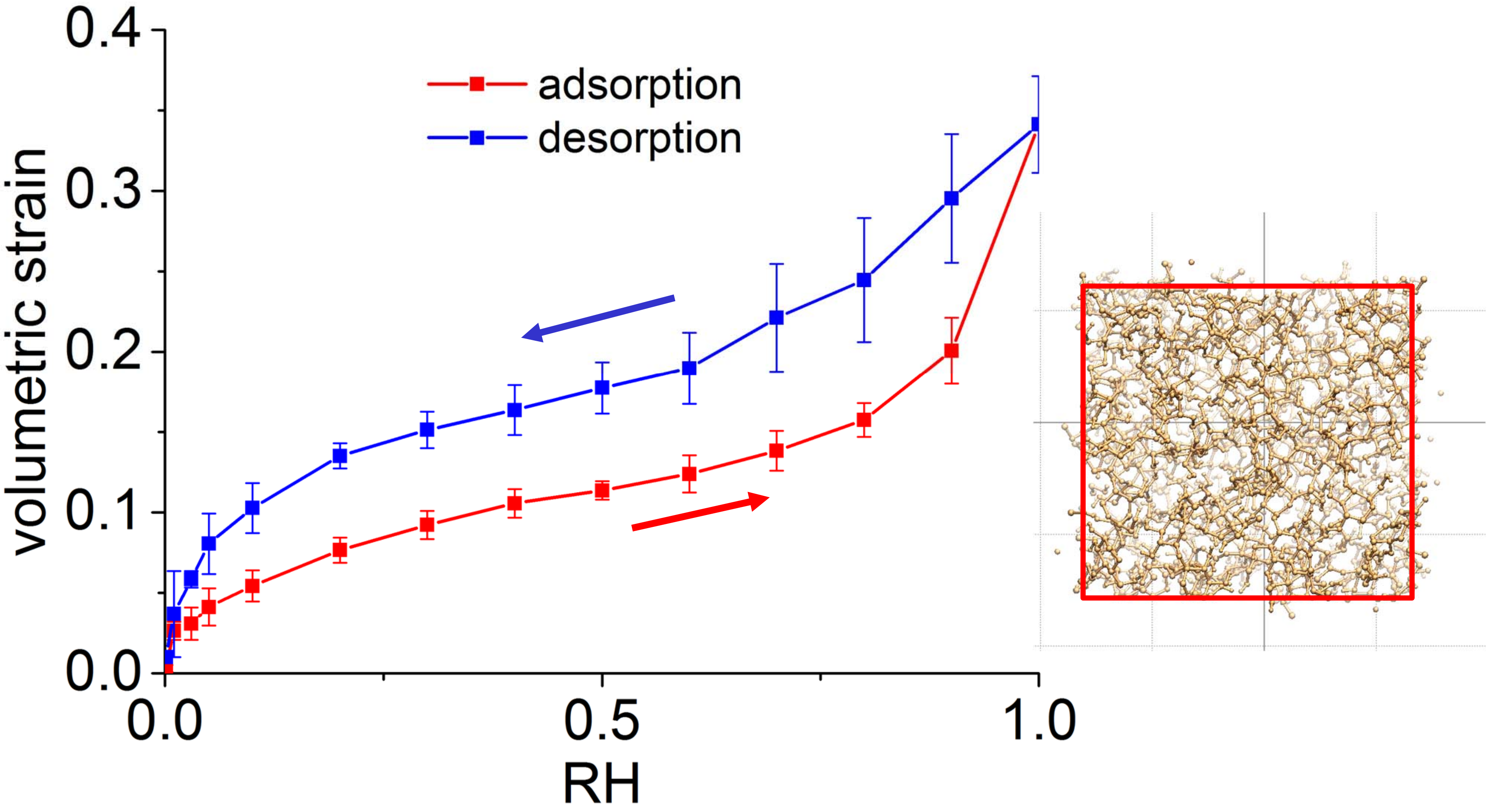
MD allows to study water configurations



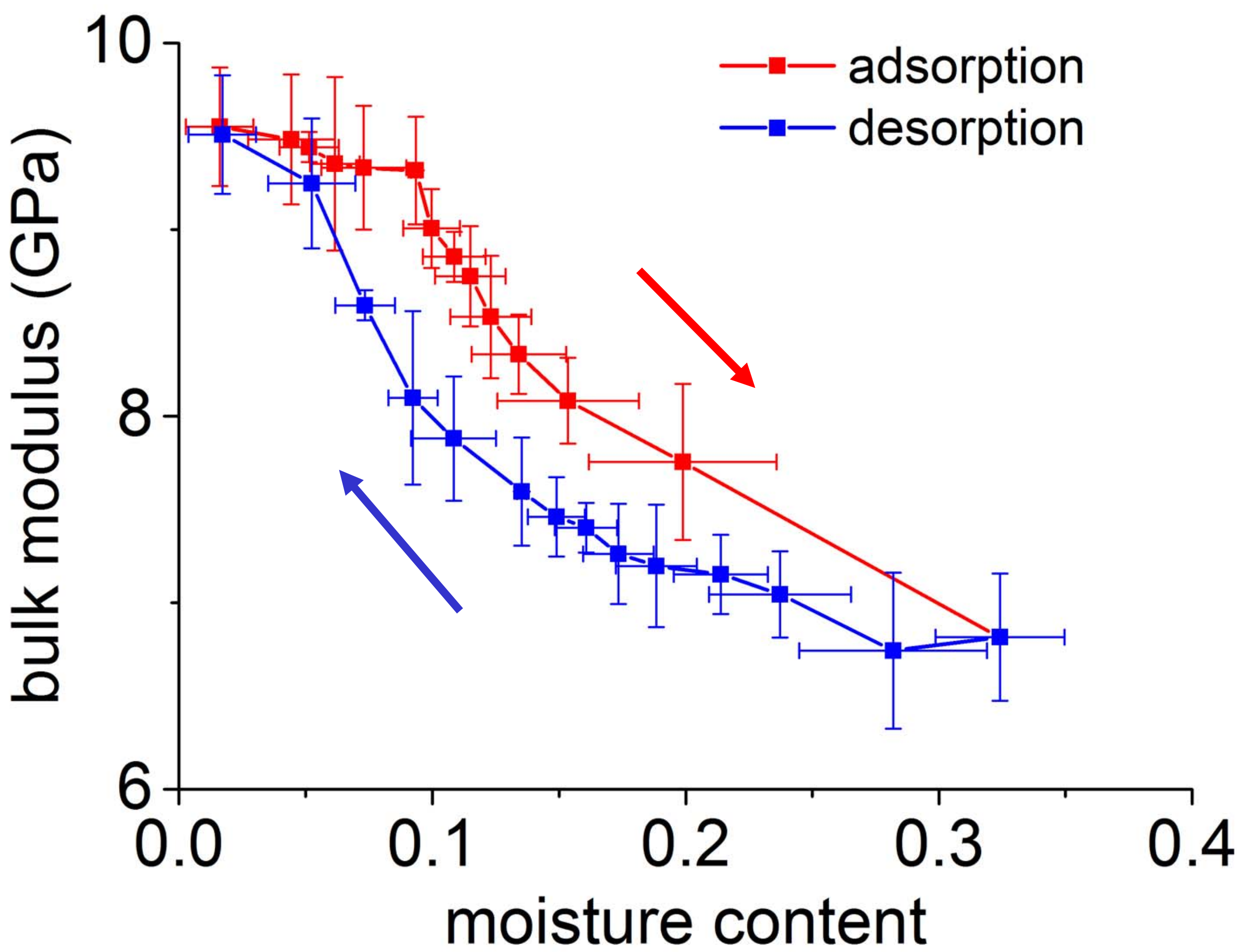
Pore filling, water molecules clustering

no surface film forming, no capillary condensation, no chemisorption

Swelling strain: hysteresis versus relative humiditity



Bulk modulus shows weakening and hysteresis

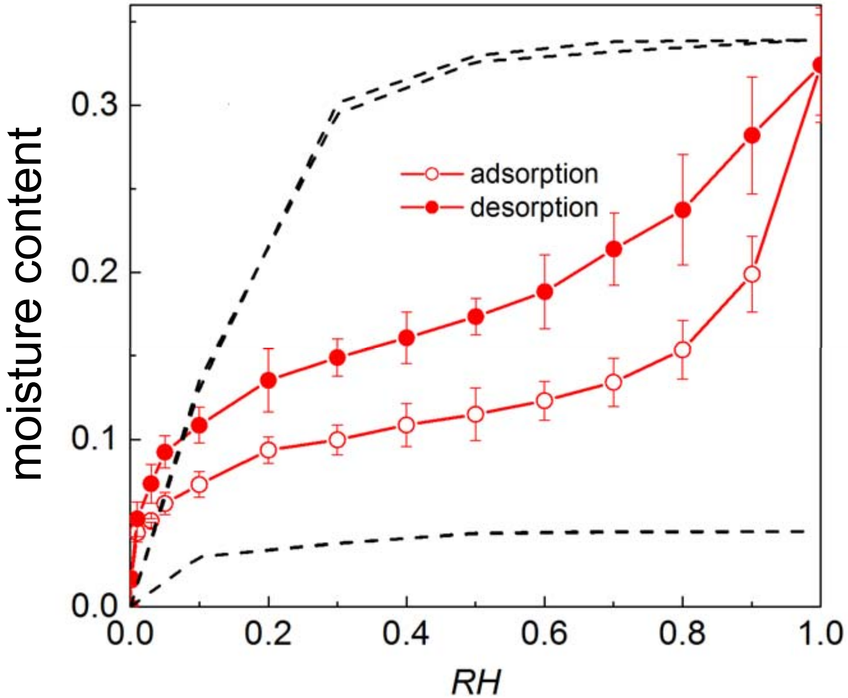


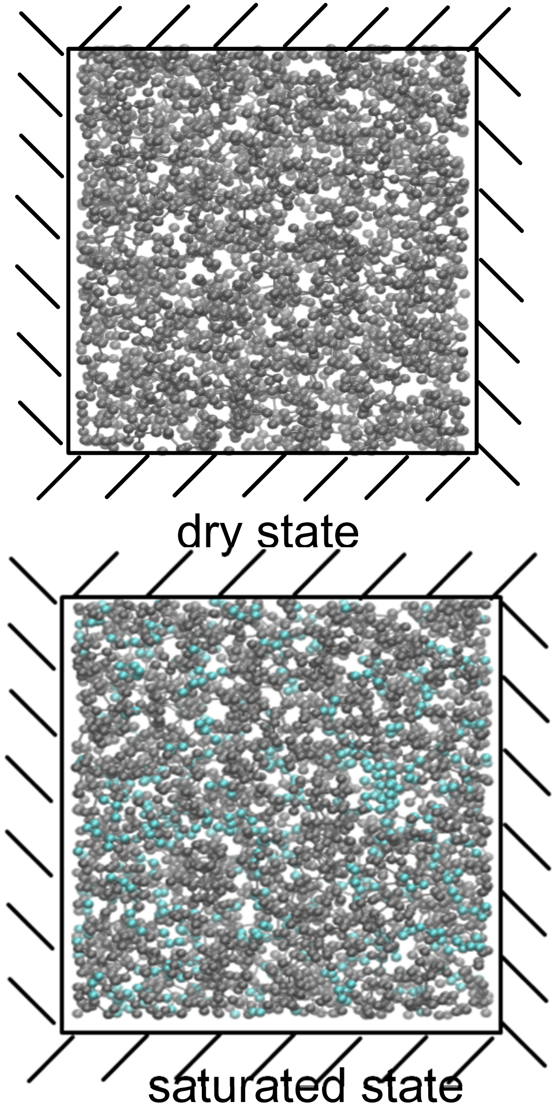
Sorption isotherm, swelling and mechanical properties show hysteresis

What is origin of hysteresis in nanoporous materials like wood ?

Results

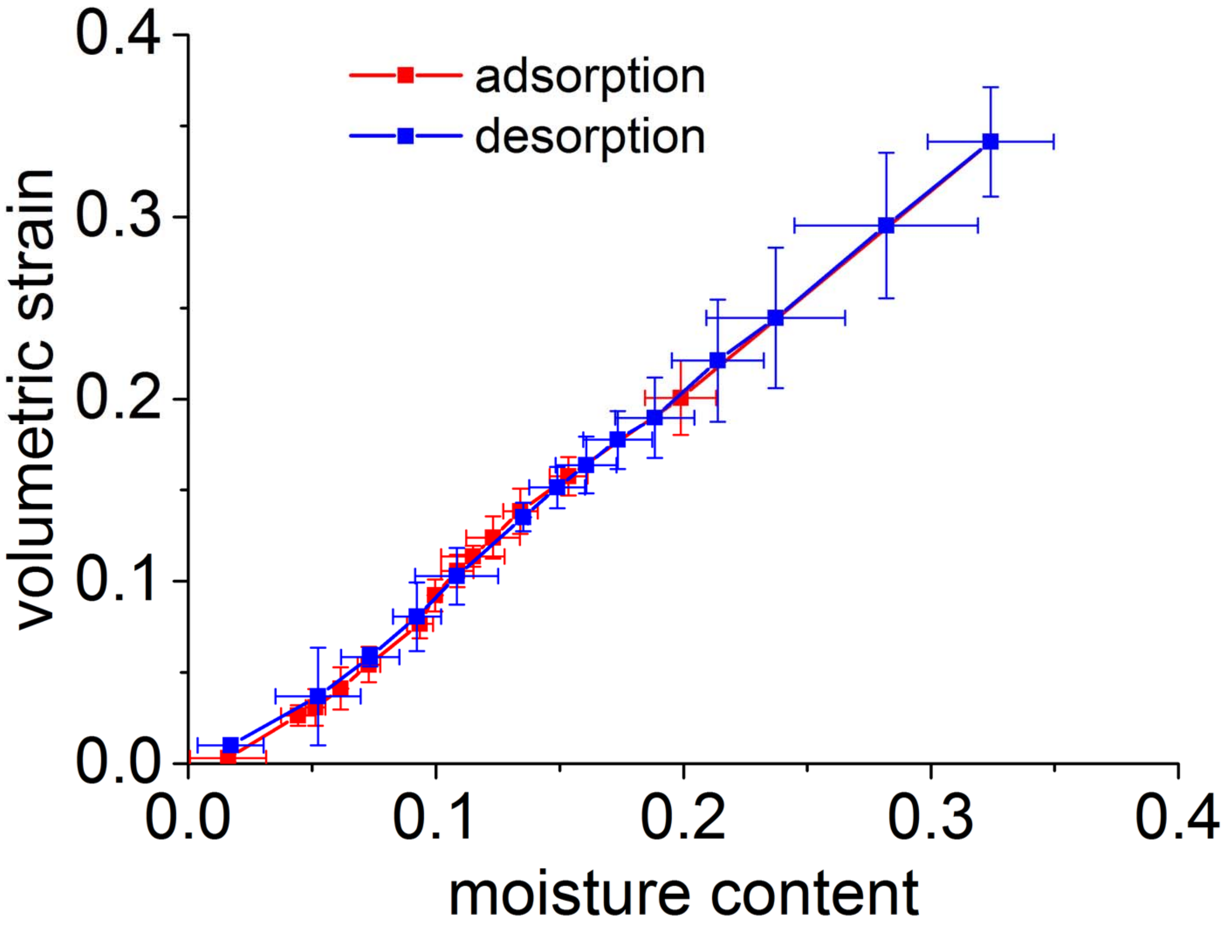
Sorption isotherms with constraints (no deformation)





Hysteresis disappears when no deformation

Swelling strain: no hysteresis versus moisture content



Swelling ~ volume of the newly adsorbed water molecules

= path independent in terms of moisture content

Confirmed by experiments

Origin of hysteresis in micro (nano) porous materials

related to the
interplay between

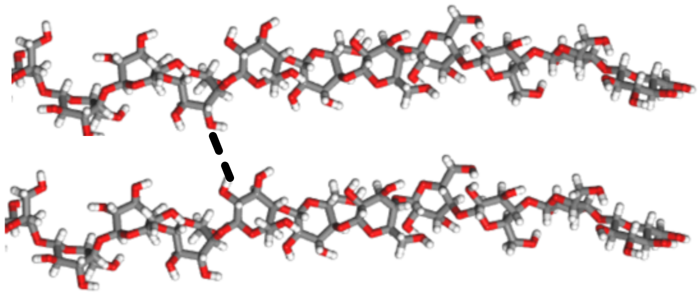
sorption - swelling

can we understand this interplay?

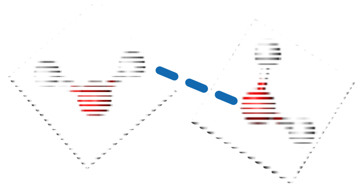
Hydrogen bonds

Different hydrogen bond (HB) types

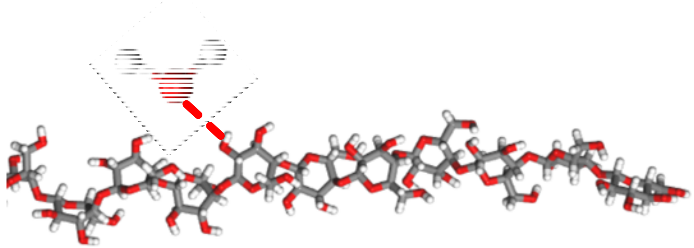
HB^{CC} :cellulose to cellulose



HB^{WW} :water to water

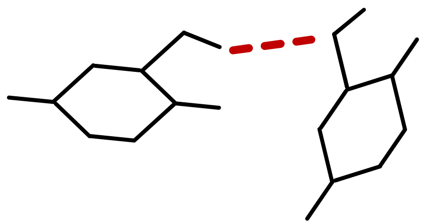


HB^{CW} :cellulose to water

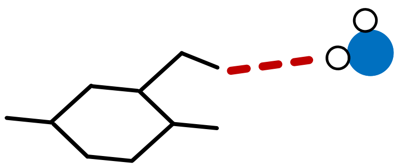


hydrogen bonds: three types

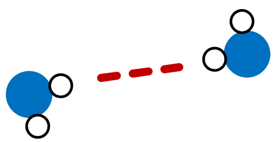
Cellulose - cellulose CC

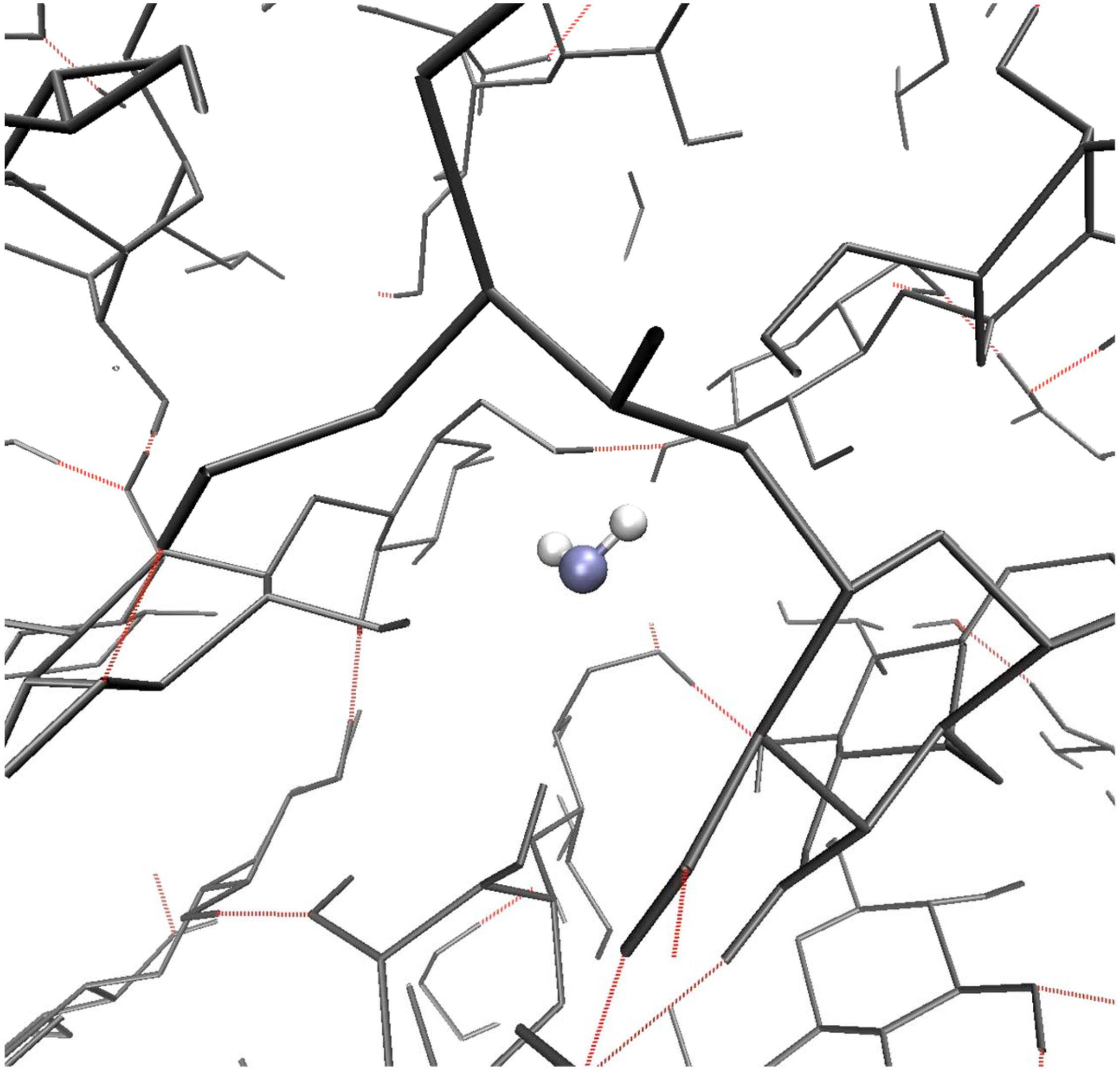


Cellulose - water: CW



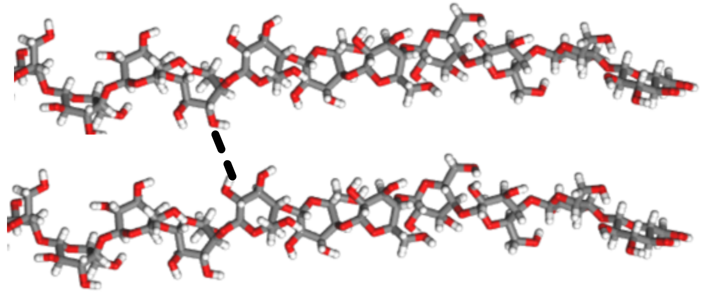
water - water: WW

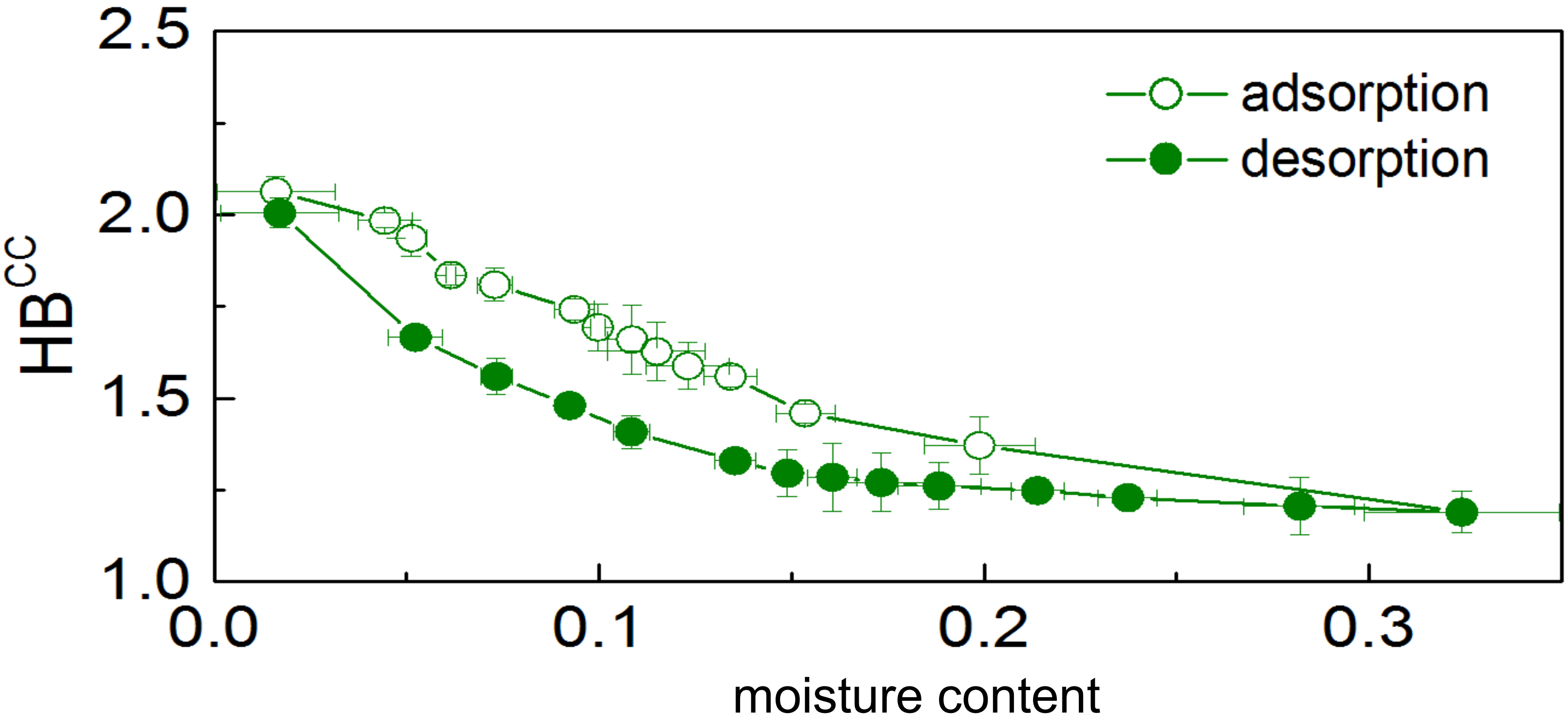




Hydrogen bonds

HB^{CC} :cellulose to cellulose



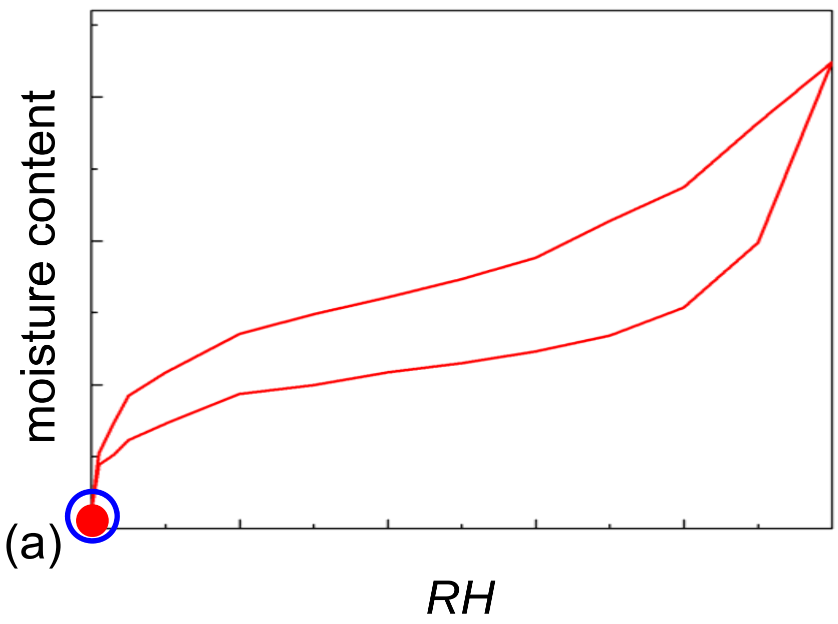


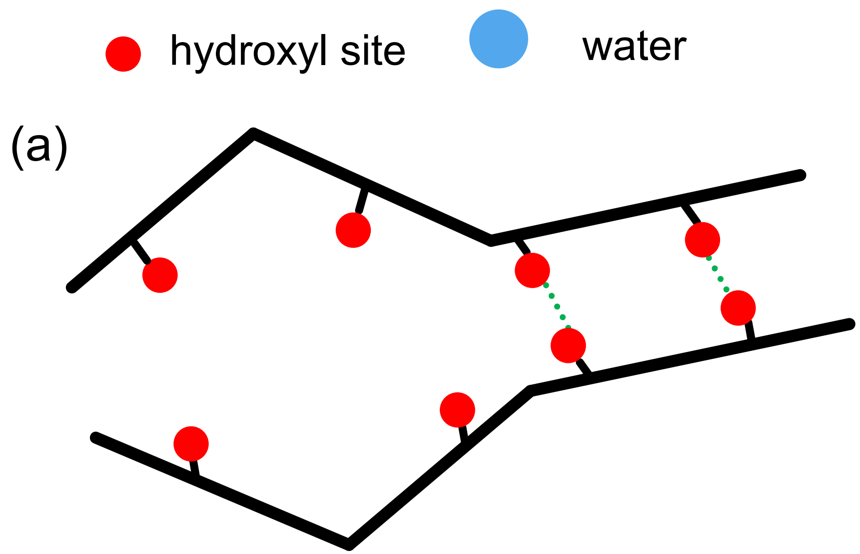
HB^{CC} breaks during swelling process

Less HB^{CC} in desorption

Hydrogen bonds

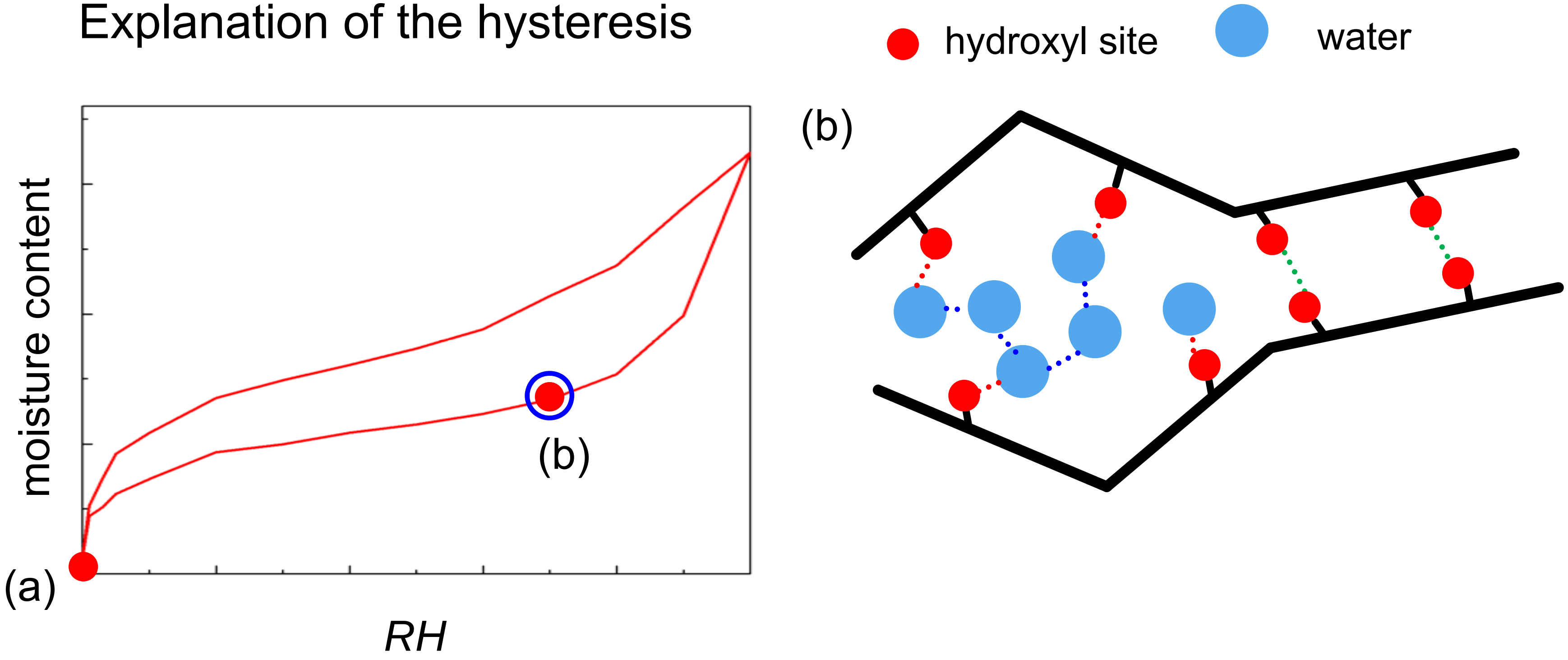
Explanation of the hysteresis





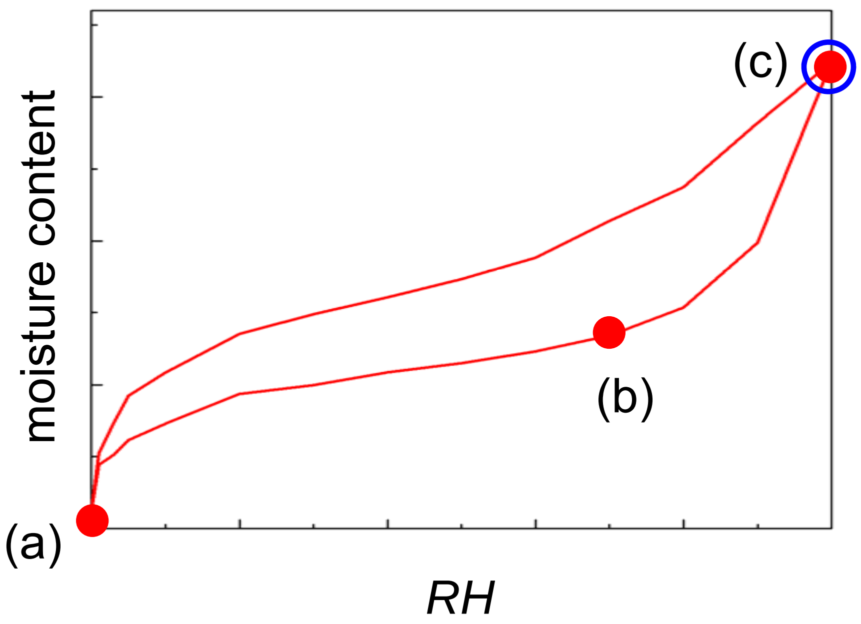
Hydrogen bonds

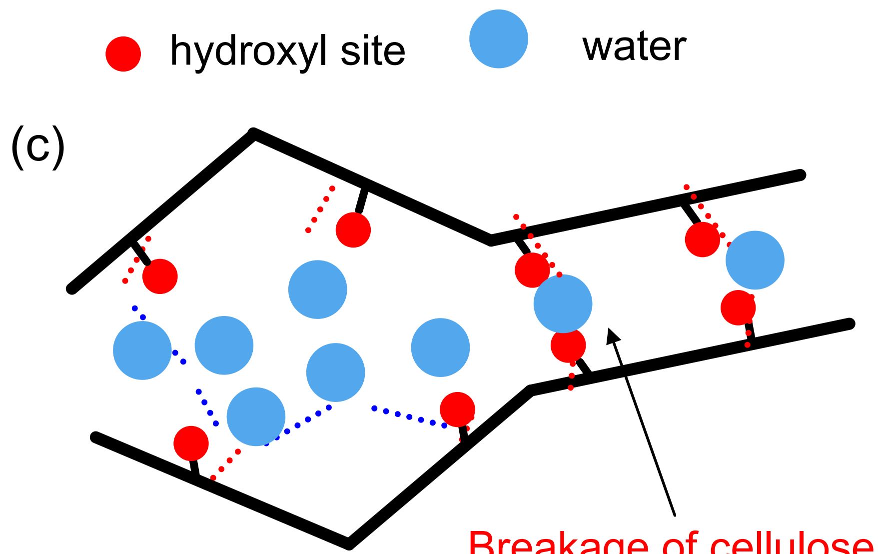
Explanation of the hysteresis



Hydrogen bonds

Explanation of the hysteresis



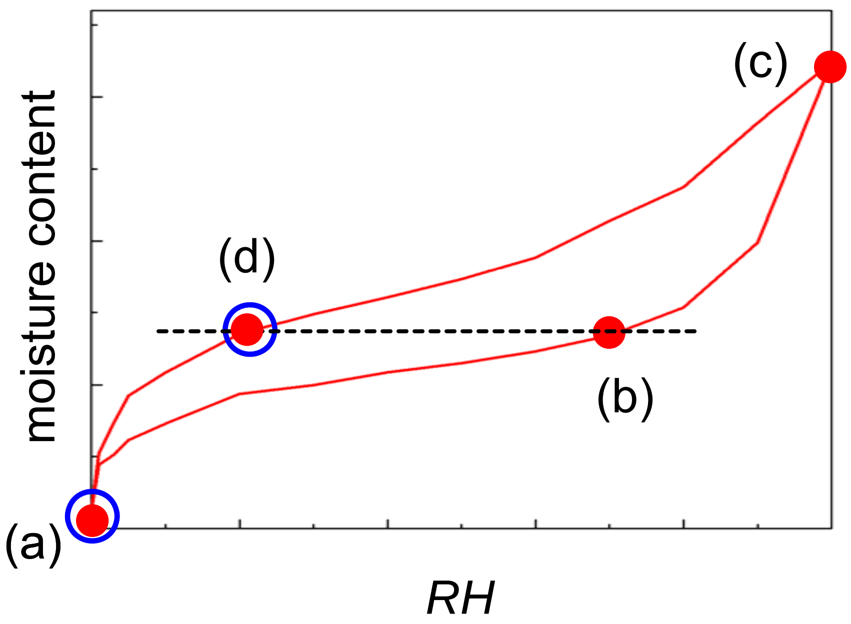


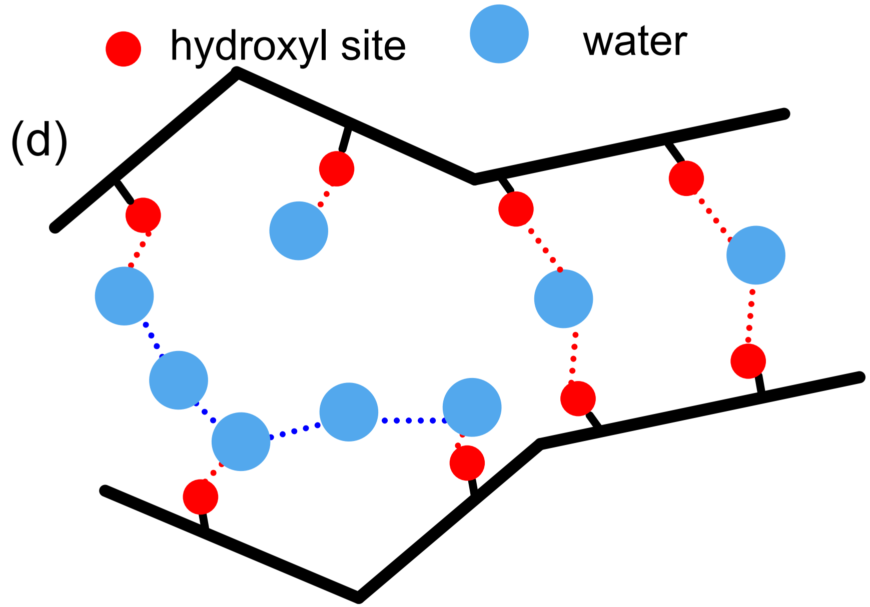
Breakage of cellulose to cellulose hydrogen bonds (HB^{CC})

Adsorption on newly exposed hydroxyl groups

Hydrogen bonds

Explanation of the hysteresis



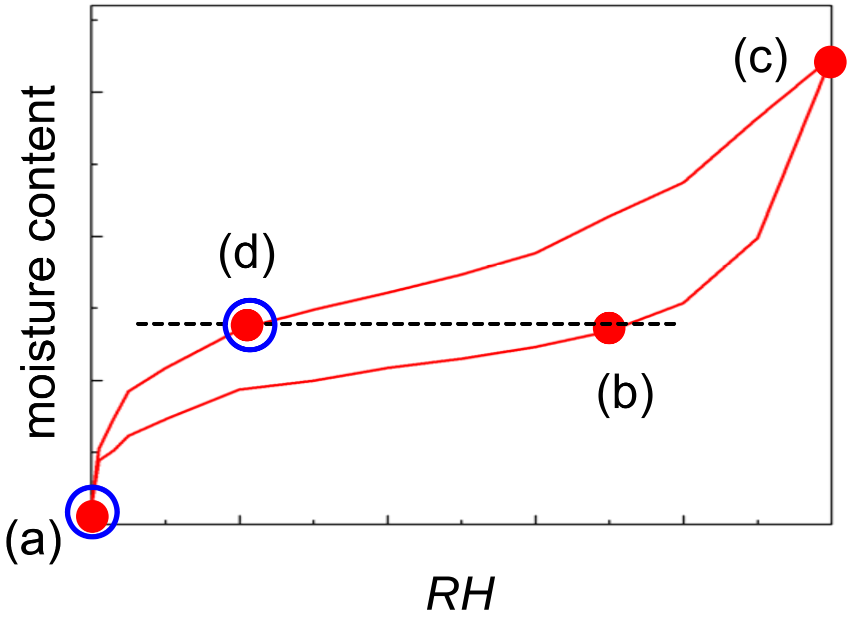


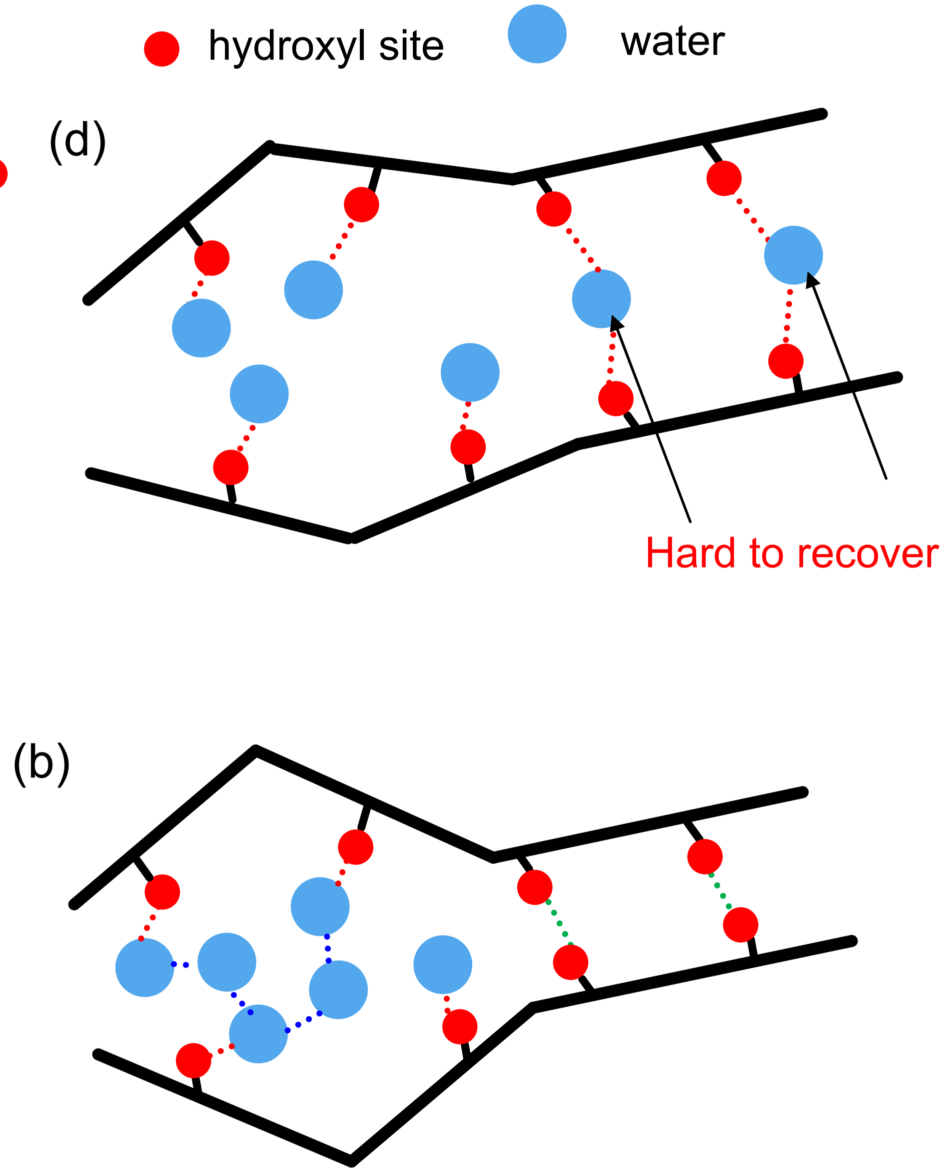
Water – water HB: lower binding energy than
cellulose – water HB binding energy

Water molecules bonded to water molecules will first desorb

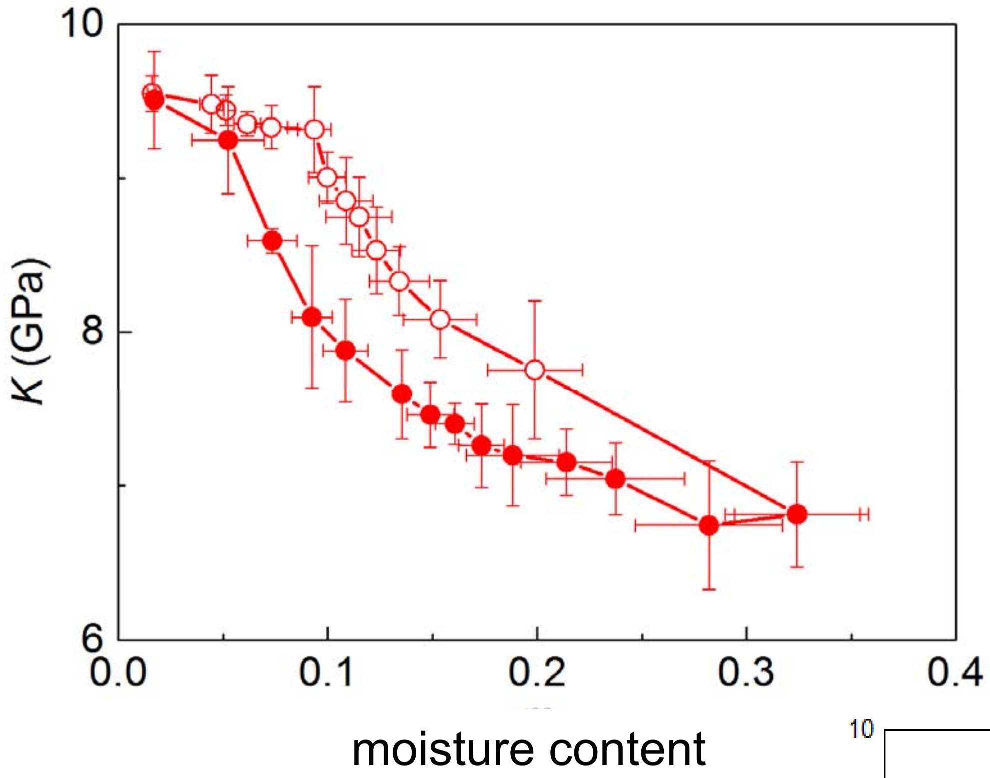
Hydrogen bonds

Explanation of the hysteresis





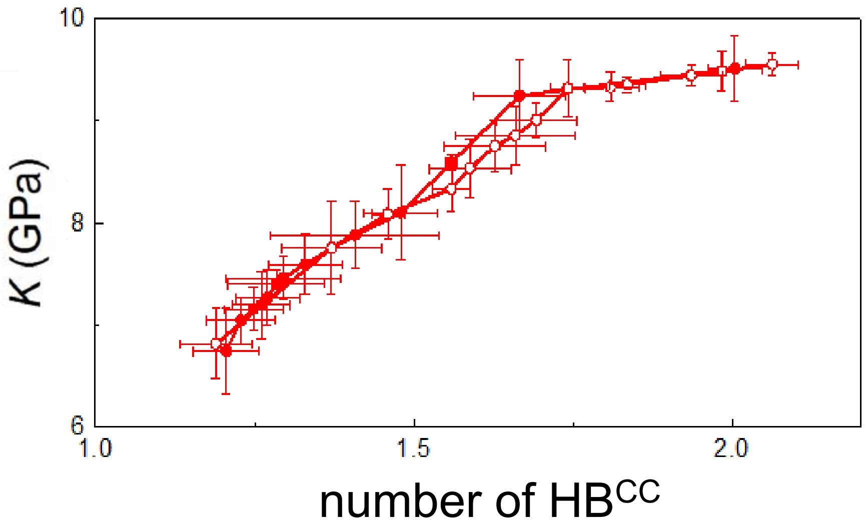
Bulk modulus



Moisture induced weakening

Hysteresis in bulk modulus

HB^{CC} controls bulk modulus



Hysteresis due to **coupling of sorption and deformation** as elucidated from different hydrogen bond (HB) distributions

Upon adsorption, **cellulose-cellulose hydrogen bonds break** due to **deformation** so that more hydroxyl sites are available to form water-cellulose hydrogen bonds.

Upon desorption, cellulose-cellulose hydrogen bonds do not reform at the same relative humidity than upon adsorption due to the **stronger binding energy of cellulose-water hydrogen** bonds compared to water-water HB.

Mingyang Chen, Benoit Coasne, Robert Guyer, Dominique Derome & Jan Carmeliet, Role of hydrogen bonding in hysteresis observed in sorption-induced swelling of soft nanoporous polymers**,**
Nature Communications, Volume 9, Article number: 3507 (2018),
https://www.nature.com/articles/s41467-018-05897-9, published Aug. 29, 2018**.**

Connected presentations:

Sorption hysteresis in wood and its coupling to swelling: a new modeling approach
Tuesday 1:30 PM, Jan Carmeliet

Understanding swelling of wood through multiscale modeling,
Tuesday 1:45 PM, Dominique Derome

New breakthrough necessary

Multiscale building physics

Some hot topics for graduate students

- **Down- and upscaling from meteorological models** to urban climate and building physics taking into account climate change
- Better understanding of origin of **heat waves**, their spatial/temporal diversity and how to **mitigate globally and locally**
- Development of **fast urban climate models** as input to building physics using proxy/surrogate models by machine learning
- Further development of **wind driven rain models**, combining them with **run-off models** and **urban drainage** models
- **Urban water management**, use of storm and gray water for UHI mitigation
- **New durability models** based on damage indicators based on coupled hygrothermal/mechanical modelling including climate change
- Better understanding of **two phase flow in porous media** at pore scale using a multiscale experimental/modelling approach

Thank you for your attention

Thanks to

Dominique Derome, Kristina Orehounig, Jonas Allegrini, Aytac Kubilay, Xiaohai Zhou, Andre Ferrari, George Mavromatidis, Hannelore Derluyn, Karol Kulasinski, Soyoun Son, Sreeyuth Lal, Christoph Waibel, Gianluca Mussetti, Feifei Qin, Pasha Piroozmand, Chi Zhang, Mingyang Chen, Lento Manickathan