1222 · 2022
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Simulation And Modeling Turbulent Spray Dynamics

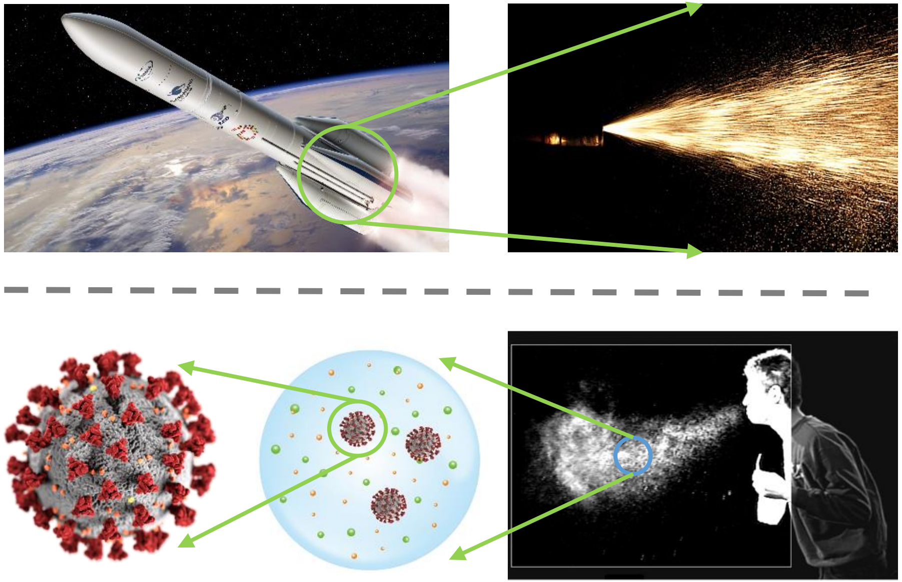
Jietuo Wang - 34th Cycle

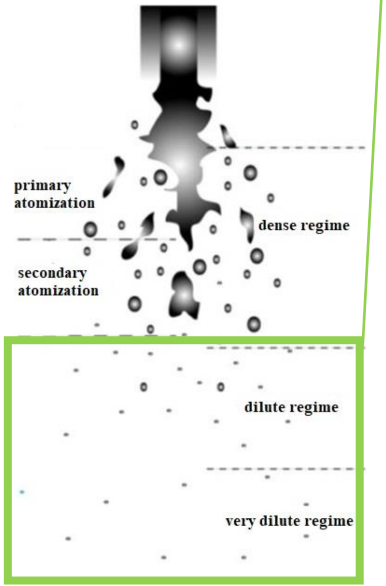
Supervisor: Prof./Dr. Francesco Picano

Admission to thesis evaluation - 15/12/2021

Motivation

- ☐ **Turbulent sprays :** Complex multiphase flows where two distinguished phases mutually interact exchanging mass, momentum and energy in a turbulent environment.





Sketch of various regimes in turbulent sprays [Jenny.2012]

☐ Diluted regime

- Dispersed droplets: **Point-droplet approximation**
- **No break-up** : surface tension >> aerodynamic forces
- **low volume fraction** ($\Phi < 10^{-3}$) : No collision / coalescence; **2-way** coupling method
- Main region occurring evaporation

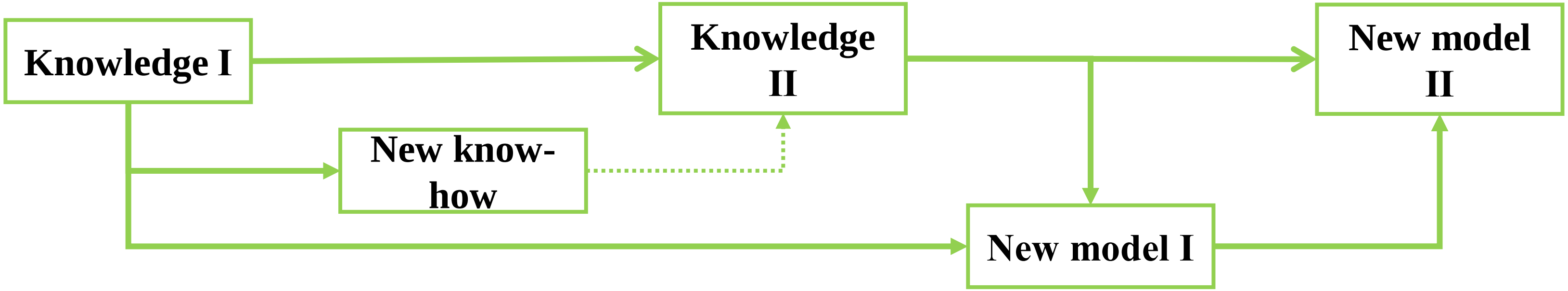
☐ Our goal

- Improve the current understanding of turbulent spray
- Apply our knowledge to solve practical issues
- Advance modeling capabilities related to turbulent spray

Research program

	1	2	3	4	5
Descr.	DNS of an evaporating turbulent diluted jet-spray at moderate Re	Modeling Lagrangian droplets within a turbulent spray with the LES method	Short-range exposure to airborne virus transmission and current guidelines	Revisiting D^2law for the evaporation of dilute droplets	Modeling the direct virus exposure risk associated with respiratory events

Flow:

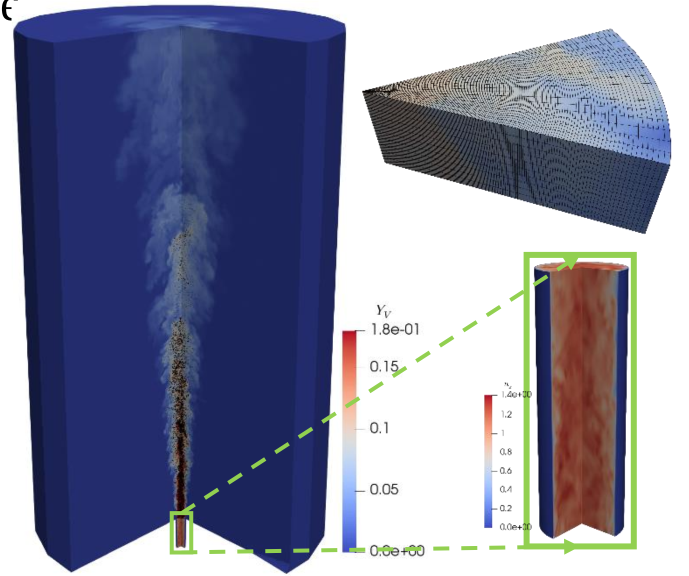


	1	2	3	4	5
Time:	*1° & 2° year*	2° year	*2° & 3° year*	*3° year*	*3° year*

Numerical tool and formulations

❑ Numerical Tool: CYCLONE

- Fully turbulent flow
- Staggered mesh
- Low Mach number NS & Point-droplet equations
- Cylindrical coordinate
- MPI parallelization



A sketch of the 3D cylindrical domain

❑ Formulations

Eulerian Gas Phase (Low Mach Navier- Stokes)	**Lagrangian dispersed phase (Point-droplet equations)**
$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\mathbf{u}) = S_m$	$\frac{d\mathbf{x}_d}{dt} = \mathbf{u}_d$
$\frac{\partial}{\partial t}(\rho Y_V) + \nabla\cdot(\rho Y_V\mathbf{u}) = \nabla\cdot(\rho\mathcal{D}\nabla Y_V) + S_m$	$\frac{d\mathbf{u}_d}{dt} = \frac{(\mathbf{u}-\mathbf{u}_d)}{\tau_d}(1+0.15\mathrm{Re}_d^{0.687})$
$\frac{\partial}{\partial t}(\rho\mathbf{u}) + \nabla\cdot(\rho\mathbf{u}\otimes\mathbf{u}) = \nabla\cdot\boldsymbol{\sigma} - \nabla P + S_p$	$\frac{dr_d^2}{dt} = -\frac{\mu_g}{\rho_l}\frac{\mathrm{Sh}}{\mathrm{Sc}}\ln(1+B_m)$
$\frac{\partial}{\partial t}(\rho E) + \nabla\cdot(\rho E\mathbf{u}) = -\nabla P\mathbf{u} + \nabla\cdot(\boldsymbol{\sigma}\otimes\mathbf{u}) - \nabla q + S_e$	$\frac{dT_d}{dt} = \frac{\mathrm{Nu}}{3\mathrm{Pr}}\frac{c_{p,g}}{c_{p,l}}\frac{T-T_d}{\tau_d} + \frac{L_v}{c_{p,l}}\frac{\dot{m}_d}{m_d}$

2-way coupling terms

$$S_m = -\sum_{i=1}\frac{dm_{d,i}}{dt}\delta(\mathbf{x}-\mathbf{x}_{d,i})$$

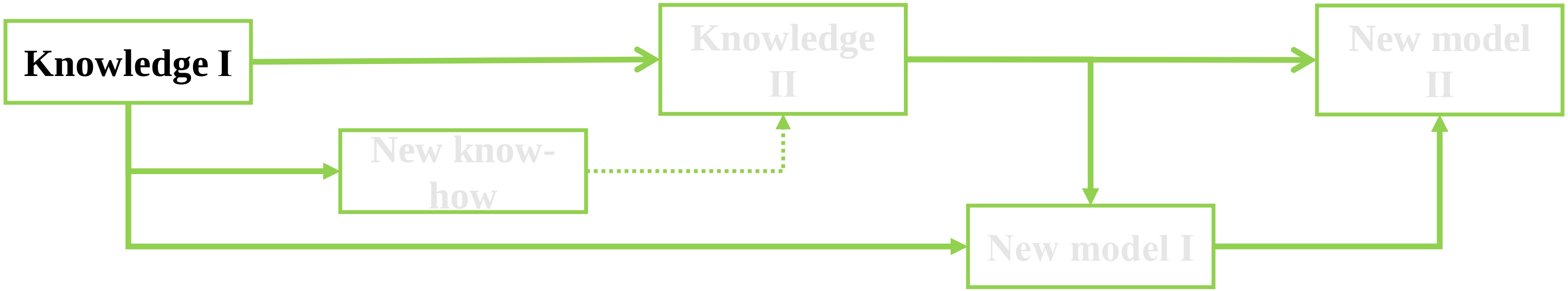
$$S_e = -\sum_{i=1}\frac{d}{dt}(m_{d,i}c_{p,l}T_{d,i})\,\delta(\mathbf{x}-\mathbf{x}_{d,i}) \qquad S_p = -\sum_{i=1}\frac{d}{dt}(m_{d,i}\mathbf{u}_{d,i})\,\delta(\mathbf{x}-\mathbf{x}_{d,i})$$

More details: Dalla Barba & Picano PRF 2018 and Wang et al. IJMF 2021

1st Project

	1	2	3	4	5
Descr.	DNS of an evaporating turbulent diluted jet-spray at moderate Re	Modeling Lagrangian droplets within a turbulent spray with the LES method	Short-range exposure to airborne virus transmission and current guidelines	Revisiting D^2law for the evaporation of dilute droplets	Modeling the direct virus exposure risk associated with respiratory events

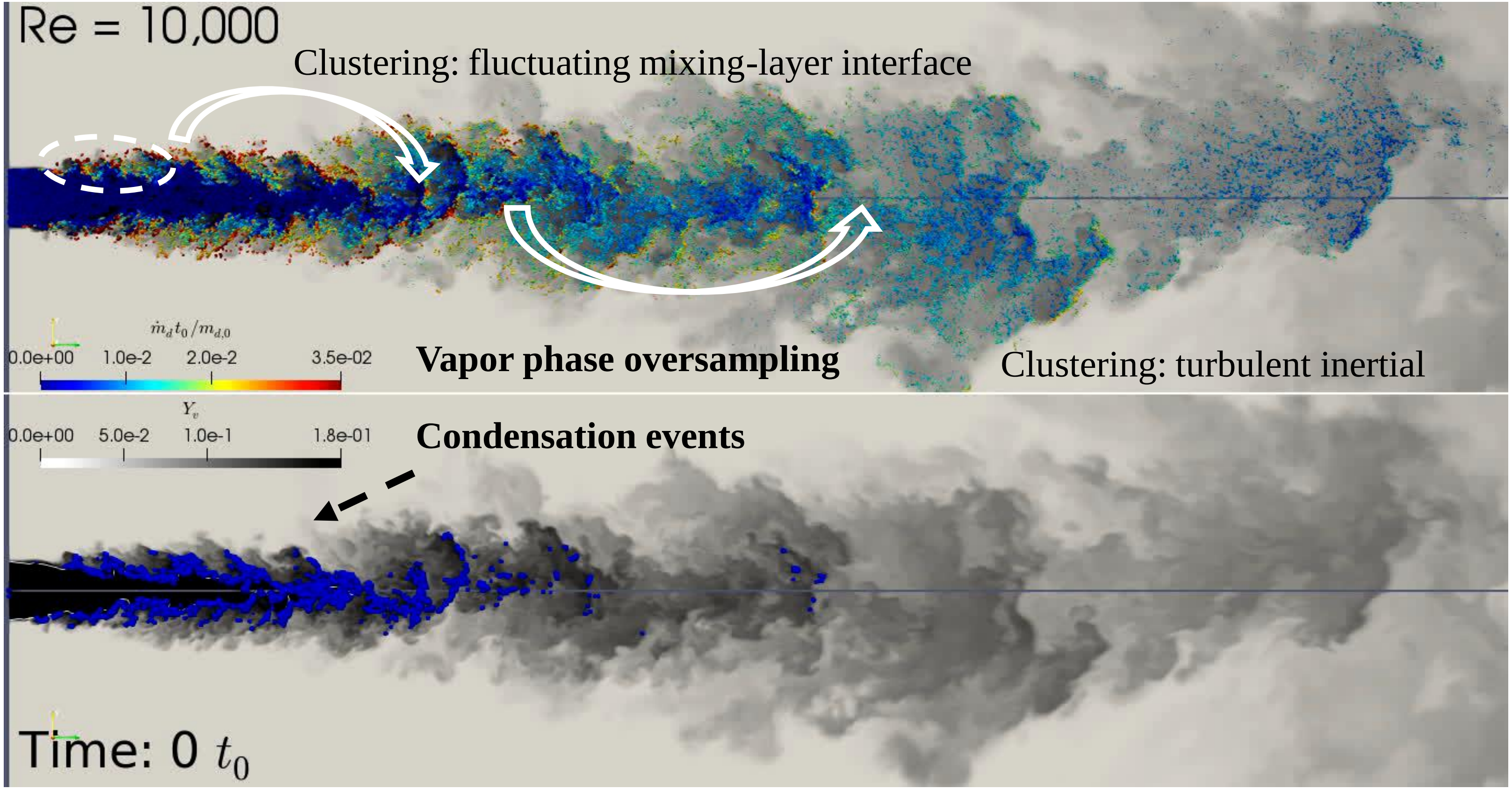
Flow:



Time:	*1° & 2° year*	2° year	*2° & 3° year*	*3° year*	*3° year*

Droplet evaporation: acetone spray

- Establishment and propagation of the preferential sampling of droplets


Re = 10,000

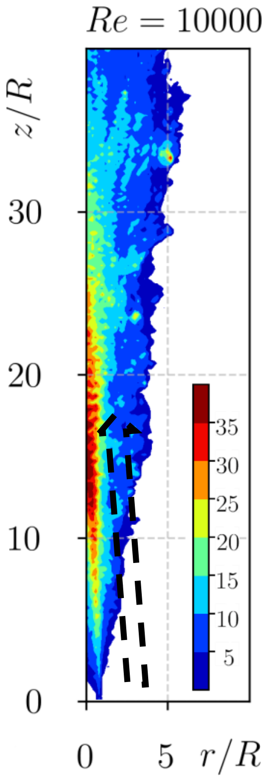
Clustering: fluctuating mixing-layer interface

Vapor phase oversampling

Clustering: turbulent inertial

Condensation events

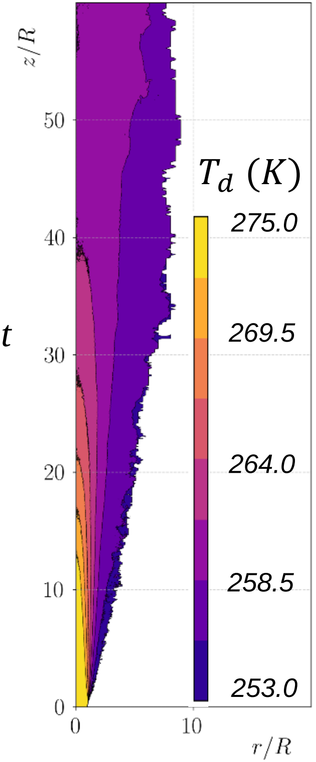
Time: 0 t_0

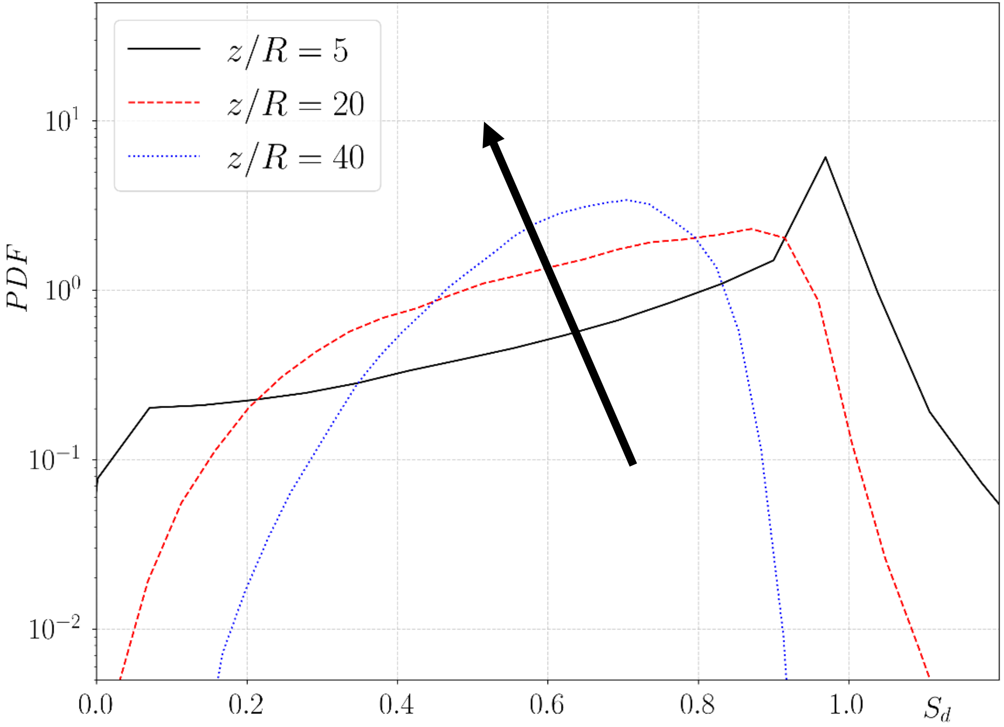


Clustering index

Droplets evaporation

Mean droplet temperature



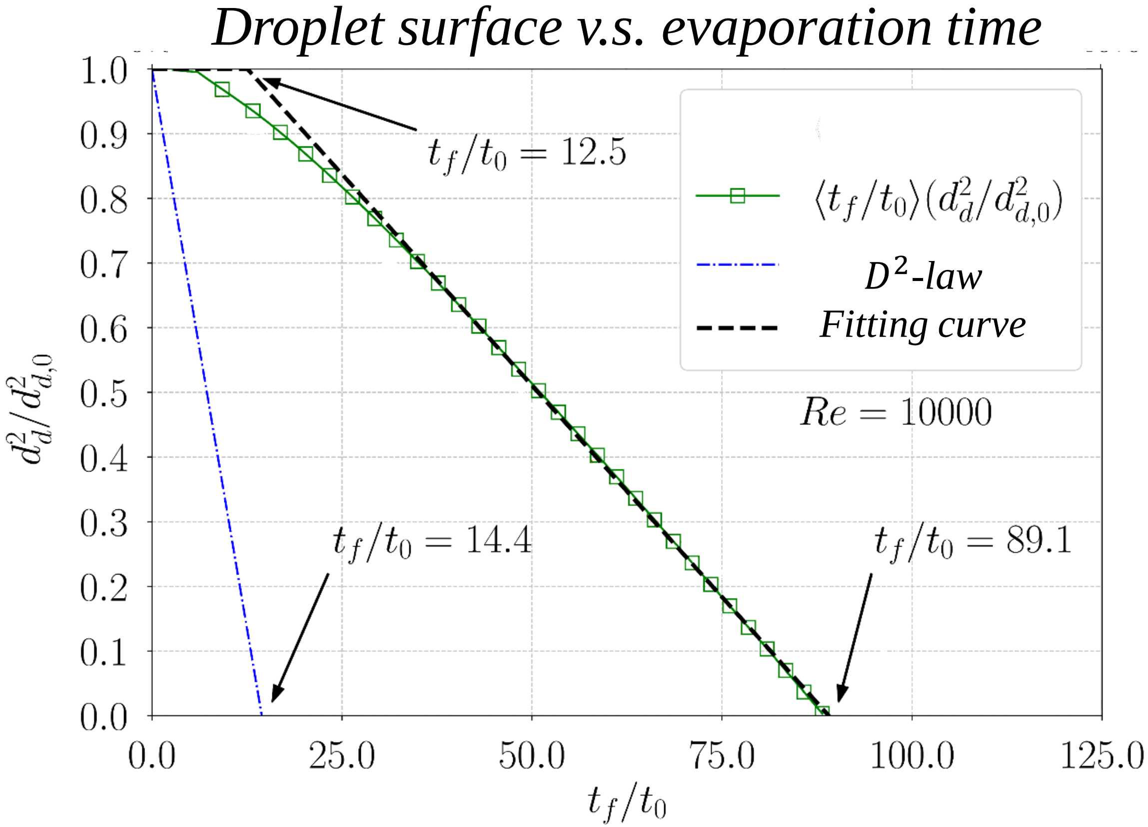


PDF of the saturation field evaluated at the droplet surface

- ➢ Lower droplet temperature w.r.t. initial value (~20 K)
- ➢ Wide distribution of saturation

Assess the D^2-law

- $\langle t_f \rangle (d_d^2/d_{d,0}^2)$: Droplets mean flight time conditioned to the square droplet diameter



- D^2-*law* is the classical and most used model for dilute evaporation: strongly underestimate droplet evaporation time.
- However, the mean droplet surface decreases in an almost linear trend, but with a small decay rate w.r.t. the classical model

➡ Project 4

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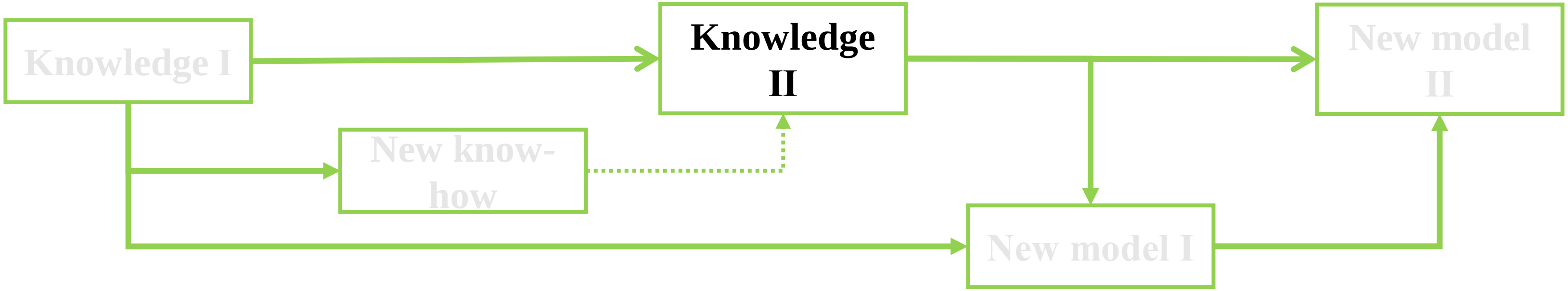
3rd Project

	1	2	**3**	4	5
Descr.	DNS of an evaporating turbulent diluted jet-spray at moderate Re	Modeling Lagrangian droplets within a turbulent spray with the LES method	Short-range exposure to airborne virus transmission and current guidelines	Revisiting D^2law for the evaporation of dilute droplets	Modeling the direct virus exposure risk associated with respiratory events
Time:	*1° & 2° year*	2° year	*2° & 3° year*	*3° year*	*3° year*

Flow:



Knowledge I

New know-how

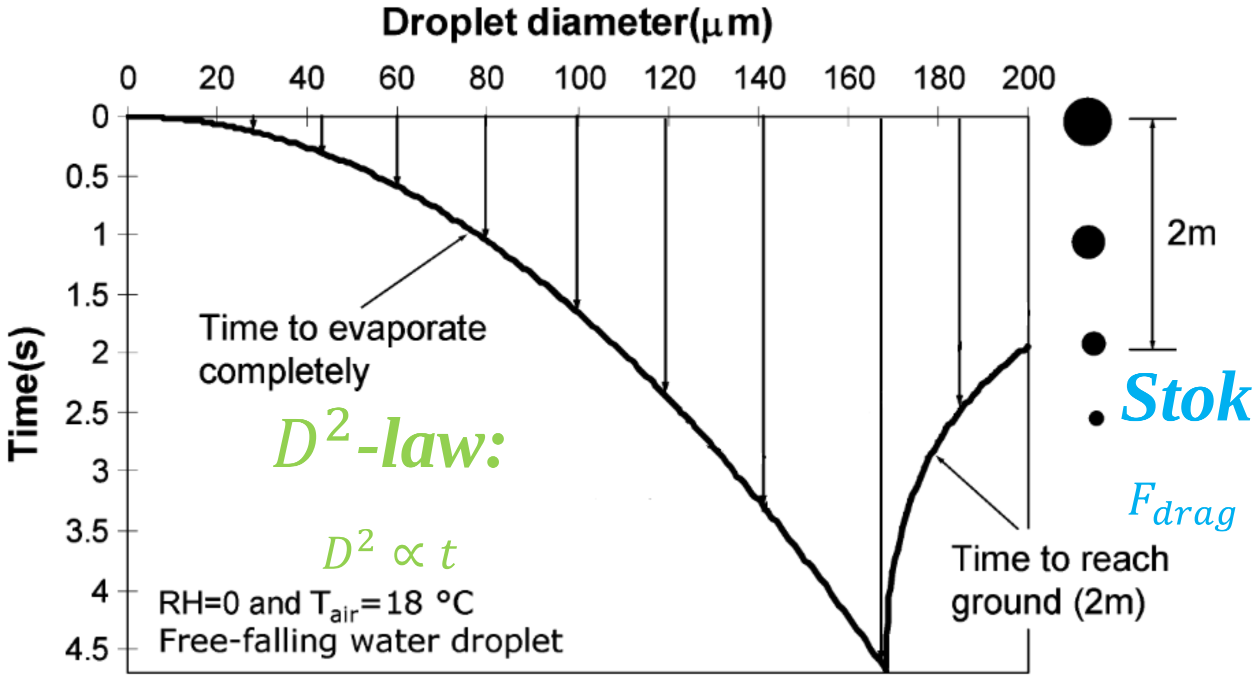
Knowledge II

New model I

New model II

Respiratoty droplets: Wells theory

The Wells evaporation-falling curve of droplets



D^2-law:

$D^2 \propto t$

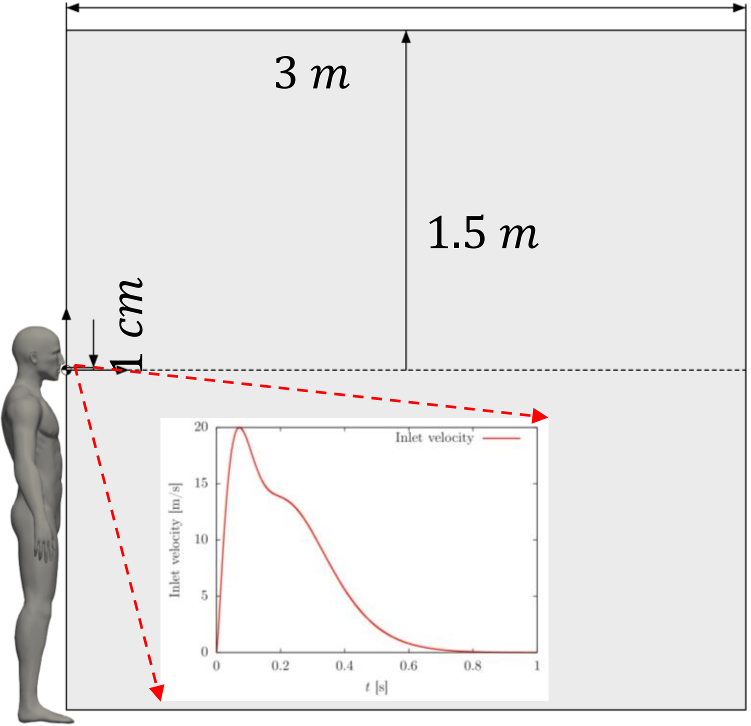
Stokes' law:

$F_{drag} \propto r_d, u_d, \mu$

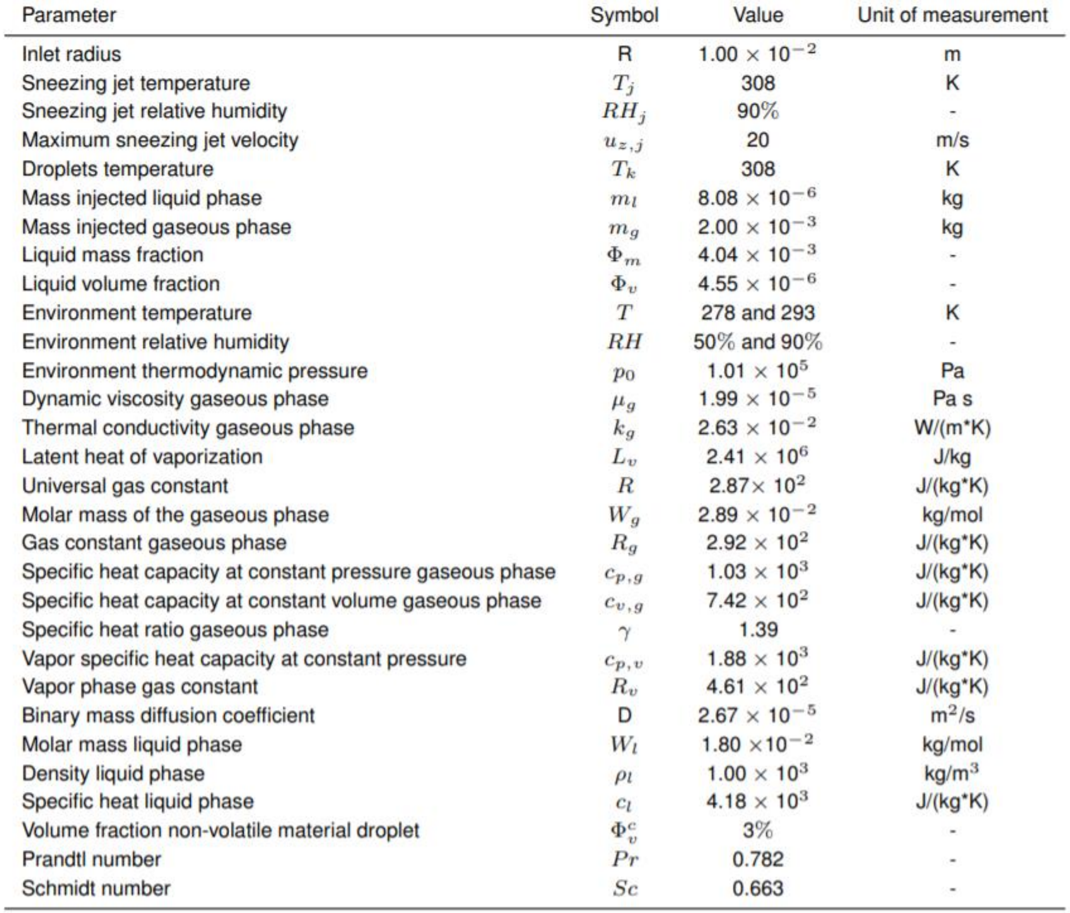
- ➢ This framework is so concise, readable and expressive that, since reported, it has been largely used in most public health guidelines, e.g. World Health Organization (WHO) and US Centers for Disease Control and Prevention (CDC).

- *Wells, W. F. (1934). Am. J. Hyg., 20, 611-18. ; Xie, X., et al. (2007). Indoor air, 17(3), 211-225; Langmuir, I. (1918). Phys. Rev. 12, 368.*

Simulation details of a sneeze



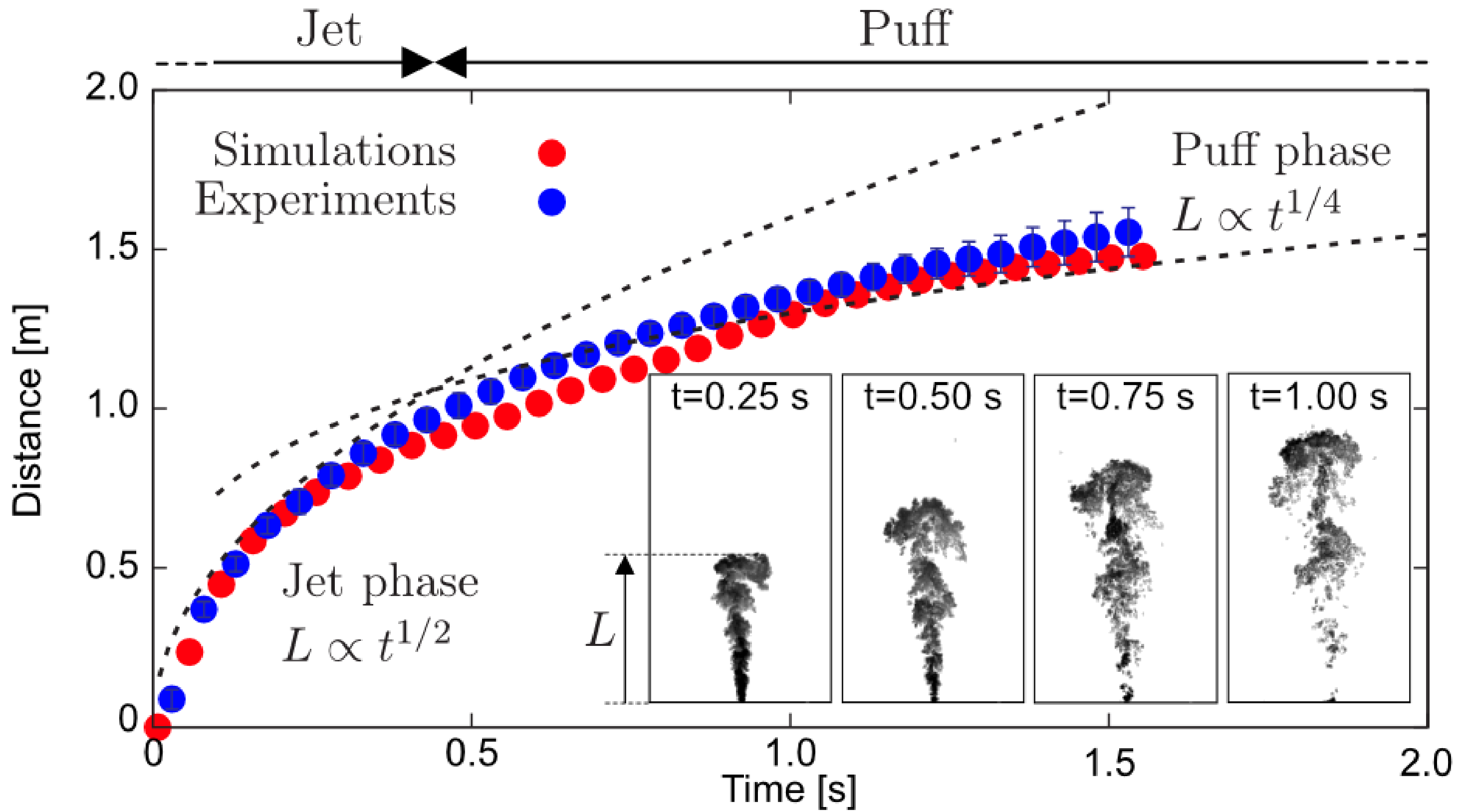
Up: sketch of the simulation setup used for the simulations;
Right: summary of the simulation parameters and thermophysical properties



Parameter	Symbol	Value	Unit of measurement
Inlet radius	R	1.00×10^{-2}	m
Sneezing jet temperature	T_j	308	K
Sneezing jet relative humidity	RH_j	90%	-
Maximum sneezing jet velocity	$u_{z,j}$	20	m/s
Droplets temperature	T_k	308	K
Mass injected liquid phase	m_l	8.08×10^{-6}	kg
Mass injected gaseous phase	m_g	2.00×10^{-3}	kg
Liquid mass fraction	Φ_m	4.04×10^{-3}	-
Liquid volume fraction	Φ_v	4.55×10^{-6}	-
Environment temperature	T	278 and 293	K
Environment relative humidity	RH	50% and 90%	-
Environment thermodynamic pressure	p_0	1.01×10^{5}	Pa
Dynamic viscosity gaseous phase	μ_g	1.99×10^{-5}	Pa s
Thermal conductivity gaseous phase	k_g	2.63×10^{-2}	W/(m*K)
Latent heat of vaporization	L_v	2.41×10^{6}	J/kg
Universal gas constant	R	2.87×10^{2}	J/(kg*K)
Molar mass of the gaseous phase	W_g	2.89×10^{-2}	kg/mol
Gas constant gaseous phase	R_g	2.92×10^{2}	J/(kg*K)
Specific heat capacity at constant pressure gaseous phase	$c_{p,g}$	1.03×10^{3}	J/(kg*K)
Specific heat capacity at constant volume gaseous phase	$c_{v,g}$	7.42×10^{2}	J/(kg*K)
Specific heat ratio gaseous phase	γ	1.39	-
Vapor specific heat capacity at constant pressure	$c_{p,v}$	1.88×10^{3}	J/(kg*K)
Vapor phase gas constant	R_v	4.61×10^{2}	J/(kg*K)
Binary mass diffusion coefficient	D	2.67×10^{-5}	m^2/s
Molar mass liquid phase	W_l	1.80×10^{-2}	kg/mol
Density liquid phase	ρ_l	1.00×10^{3}	kg/m^3
Specific heat liquid phase	c_l	4.18×10^{3}	J/(kg*K)
Volume fraction non-volatile material droplet	Φ_v^c	3%	-
Prandtl number	Pr	0.782	-
Schmidt number	Sc	0.663	-

Jietuo WANG

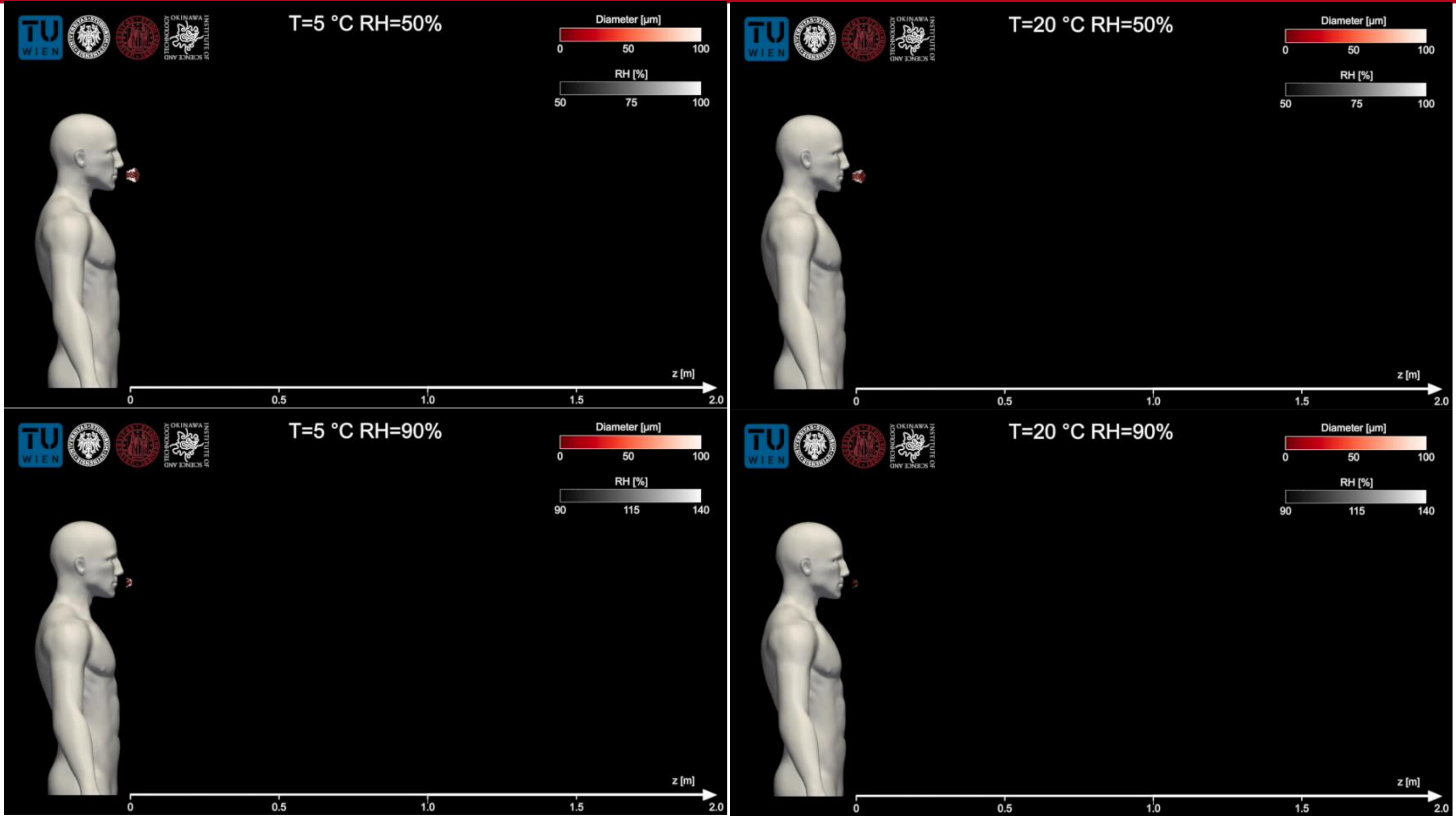
Simulating sneeze: validation



Distance traveled by the front of the jet: comparison between simulations and experiments. (Insets) Qualitative visualizations obtained from experiments showing the jet/puff evolution.

- Two different phases of propagation: jet phase & puff phase. → Project 5
- Both simulations and experiments exhibit a very similar behavior and are in excellent agreement.

Qualitative visualizations



Size threshold used in public guidelines to differentiate large droplets and aerosols : $5\mu m$?

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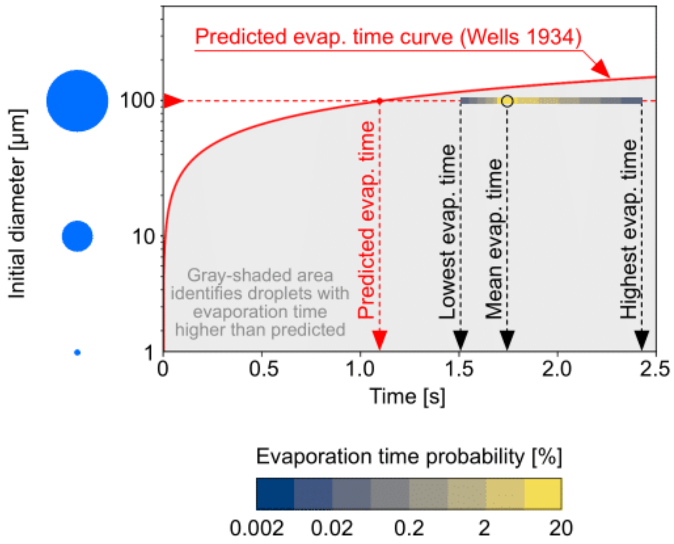
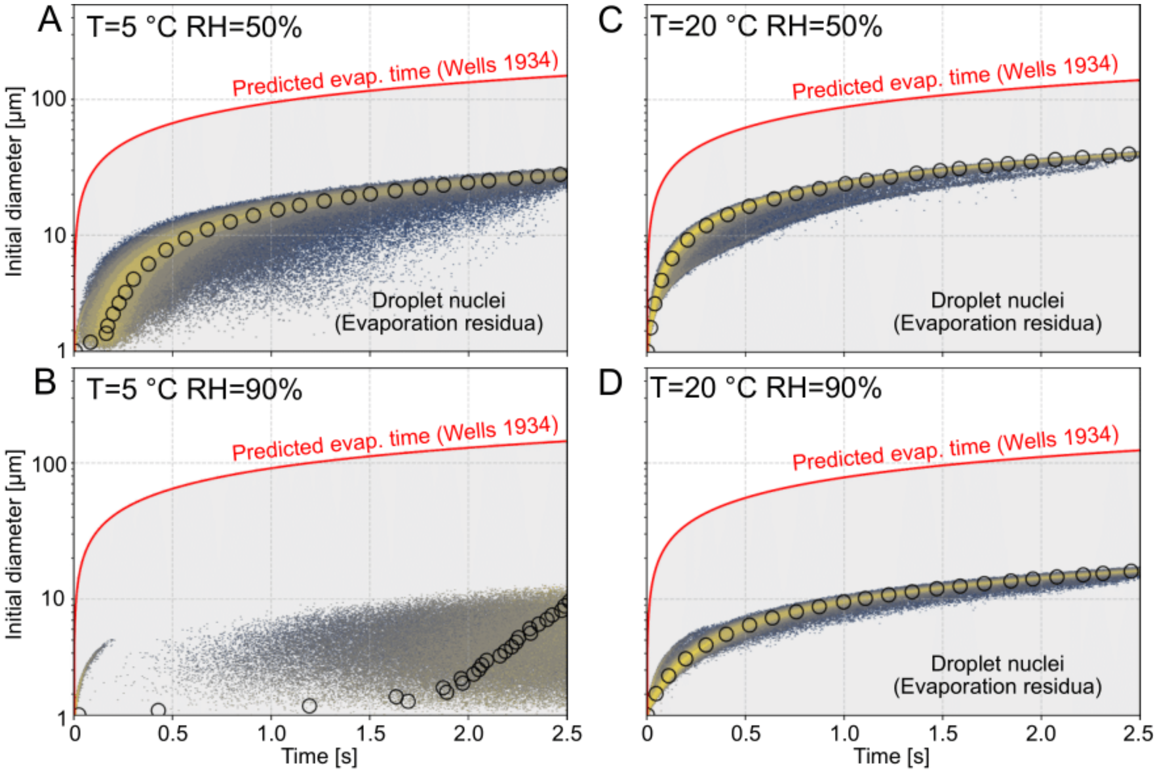
Respiratory droplets: lifetime *v.s.* size

Time required by the respiratory droplets to complete the evaporation process in the four ambient conditions tested.

Sample plot (100 μm droplets)





- ➢ Droplets' lifetime is always about <u>one order of magnitude larger</u> compared to previous predictions by Wells theory, in some cases up to 200 times. (some universality) → Project 4

W. F. Wells (1934). Am. J. Hyg., 20:611–618.

4th Project

	1	2	3	4	5
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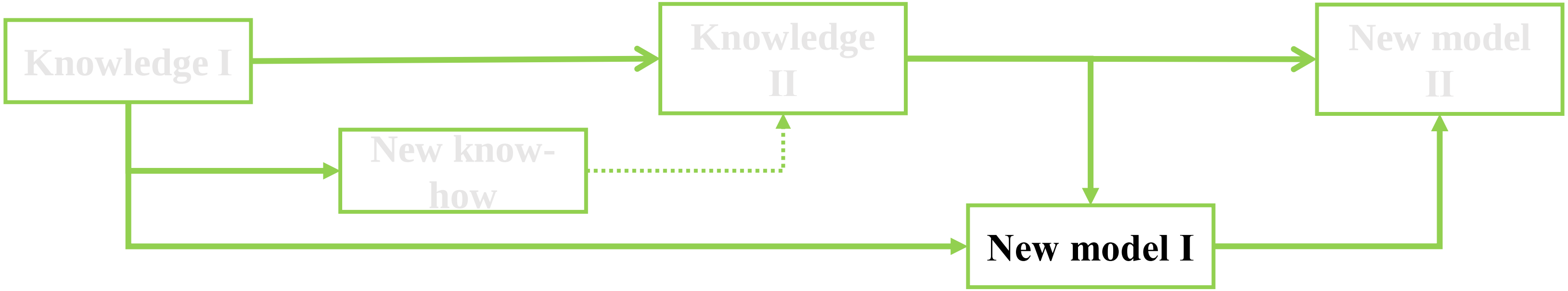
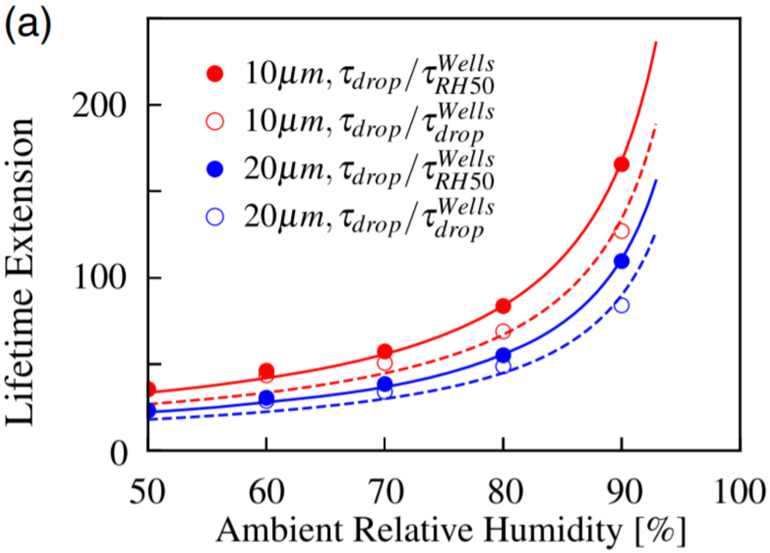
Flow:

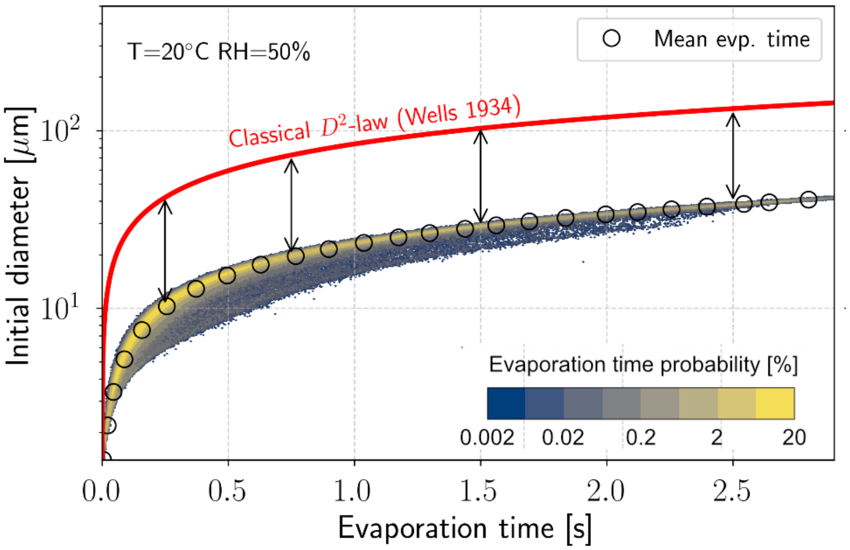


Time:	*1° & 2° year*	2° year	*2° & 3° year*	*3° year*	*3° year*

Extended lifetime of respiratory droplets



Extended lifetime of respiratory droplets as a function of relative humidity up to $RH = 90\ \%$



Evaporation time of respiratory droplets

- Chong et al. showed that *"…droplets have* $O(100)$ *longer lifetimes in a turbulent vapor puff at high ambient relative humidity than that predicted by the Well theory…"*. Our results confirm this observation.
- Although the resulting evaporation times are much larger than D^2-law/Wells predictions, it is worth observing that the D^2-law scaling seems to still bear some universality.

- *W. F. Wells(1934). Am. J. Hyg., 20:611–618, 1934; K. L. Chong et al. (2021). Phys. Rev. Lett. 126, 034502 (2021)*

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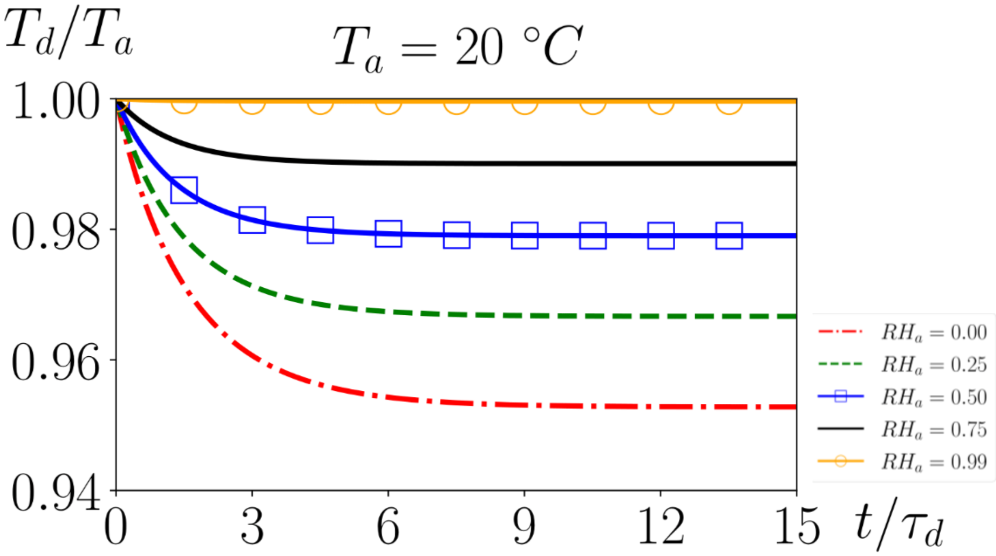
D^2-law: a revision (very dilute regimes)

Formulations for droplet evaporation

<table>
<tr><th>Full coupling</th><th>Classical D^2law</th><th>Revised D^2law</th></tr>
<tr><td colspan="3">$\frac{dr_d^2}{dt} = -K$</td></tr>
<tr><td colspan="3">$K = \frac{Sh}{Sc}\frac{\rho_g}{\rho_l}\nu_g H_m[T_d]$</td></tr>
<tr><td rowspan="2">$T_d[t]$</td><td colspan="2">$T_d \equiv T_{d,0}$</td></tr>
<tr><td>$\equiv T_{g,0}$</td><td>$\equiv T_{g,0} - \frac{Sh\ Pr\ L_v}{Nu\ Sc\ C_{p,g}} H_m$</td></tr>
</table>

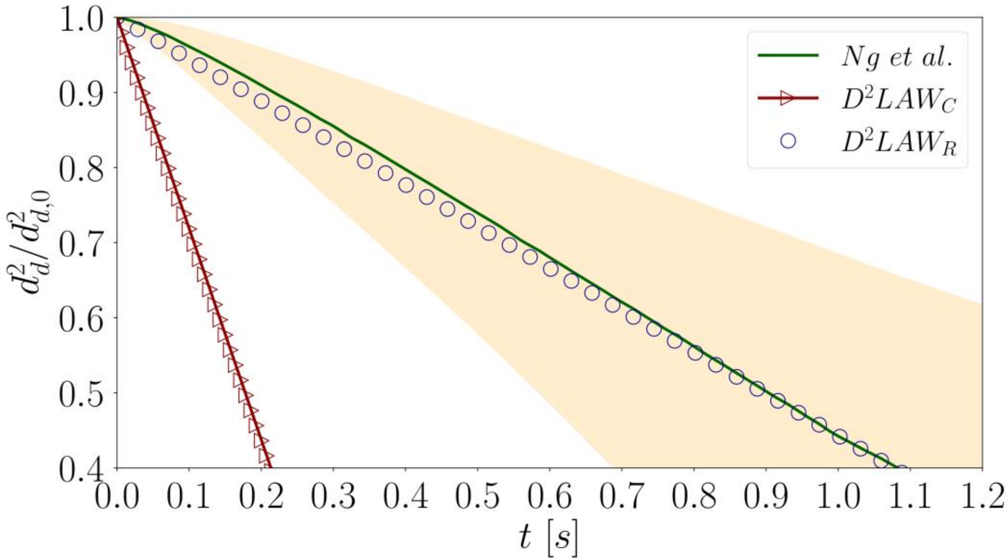


Temporal evolution of the temperature of evaporating water droplets, T_d, at T_a=20°C.

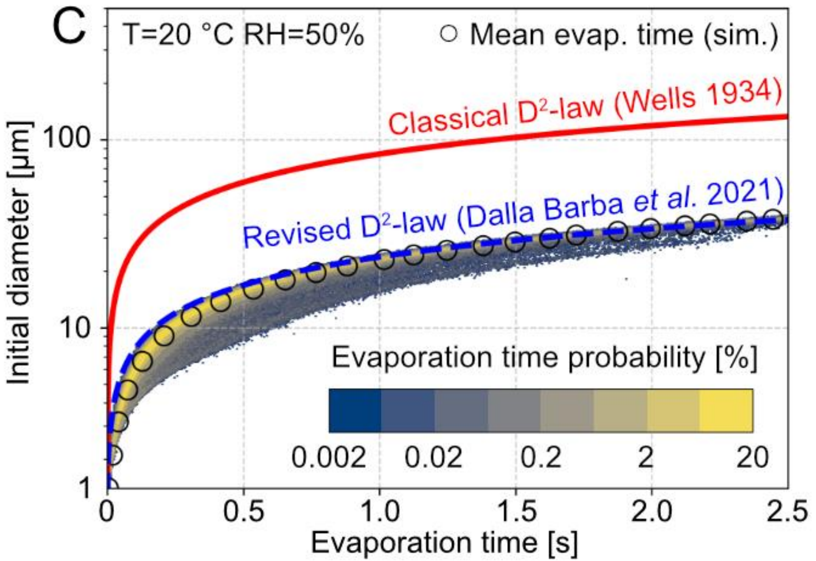
- In our revised D^2-law the droplet temperature is assumed constant but equal to asymptotic equilibrium **accounting for latent heat**
- **K** for $T_a = 20°C$ & $RH_a = 50\% \rightarrow K_c = 4.4 \times 10^{-10}$ **;** $K_r = 1.4 \times 10^{-10}$

Test the revised D^2-law in respiratory jet

Coughing(*Ng et al.)*



Sneezing(*Wang et al.)*



- The proposed model is capable to accurately predict the mean evaporation behaviors of respiratory droplets with respect to the traditional D^2-law /Wells theory.

- *Ng, C. S. et al. (2021). Phys. Rev. Fluids, 6(5), 054303.*

5th Project

	1	2	3	4	5
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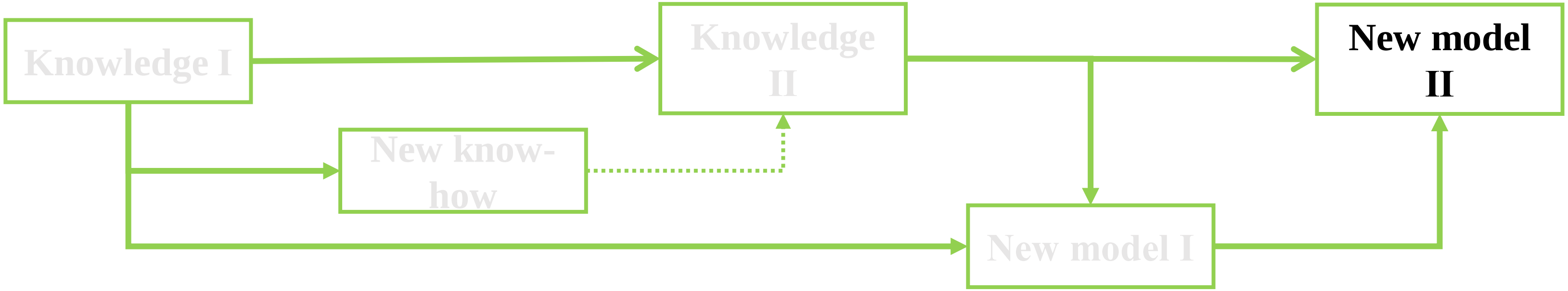
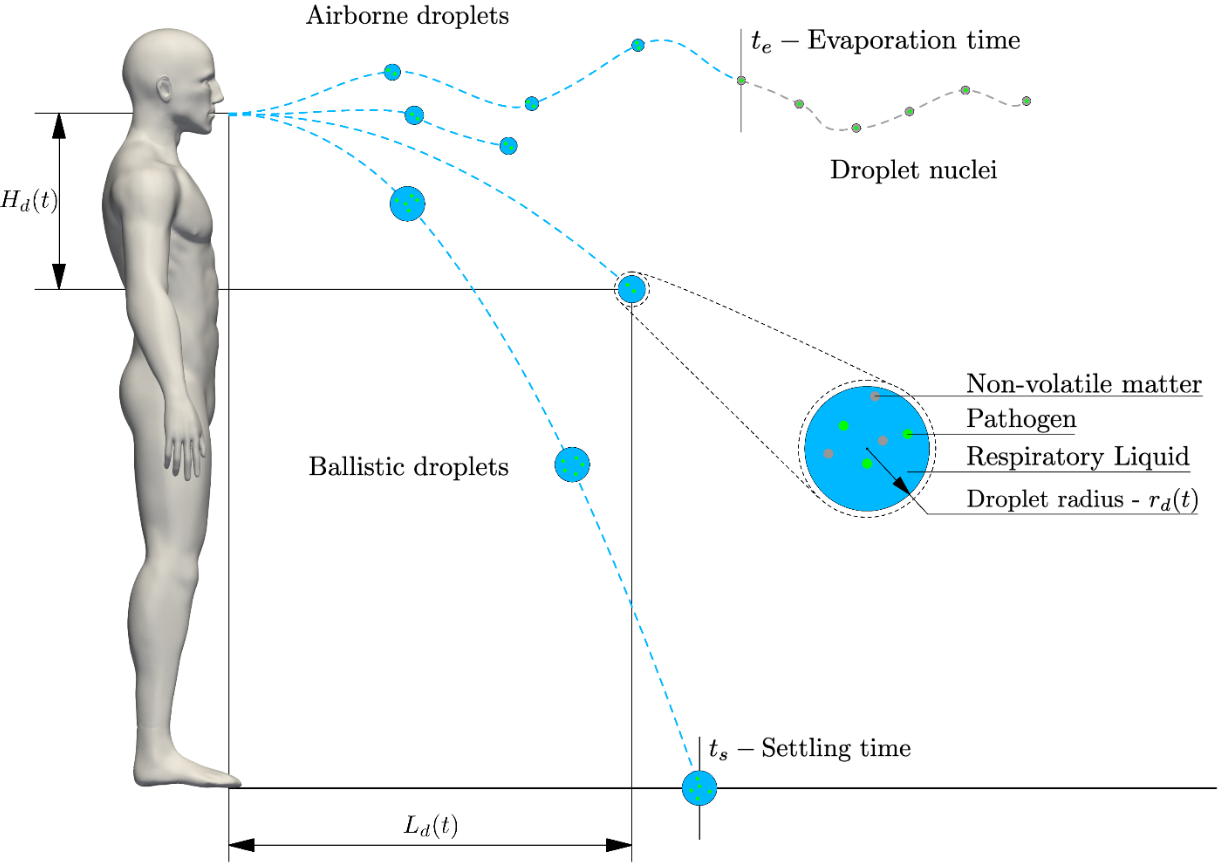
Time:	*1° & 2° year*	2° year	*2° & 3° year*	*3° year*	*3° year*

Flow:



A new framework for respiratory droplets



➢ Our model includes:

1. a revised D^2-law;
2. a correction to Stokes law;
3. the two-stage propagation of respiratory events: jet & puff.

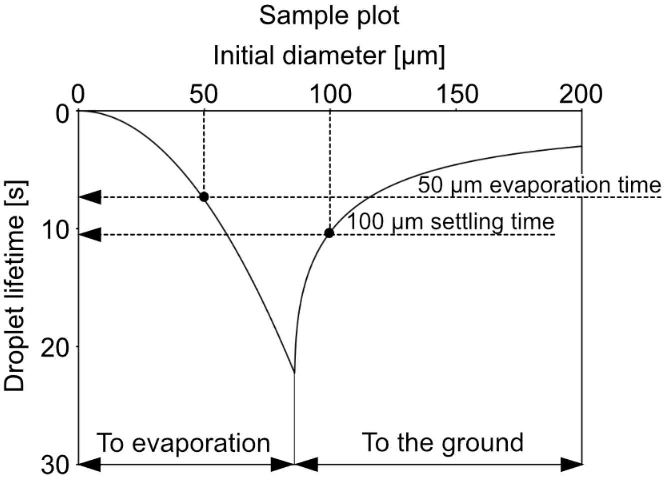
$$t_l = \min(t_e, t_s)$$

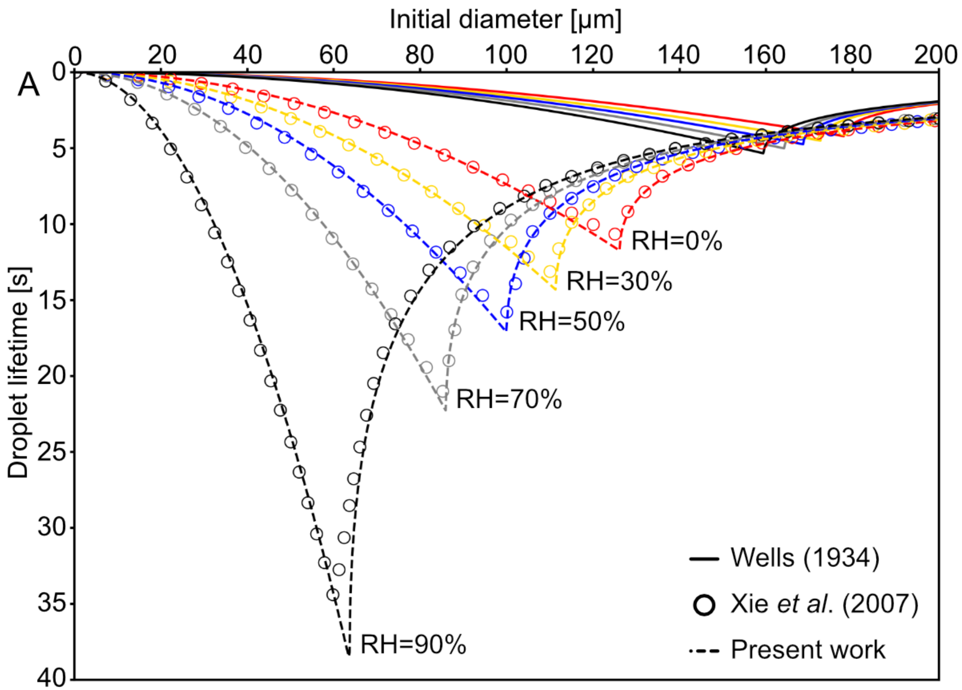
$$t_e = \frac{D_{d,0}^2}{k}$$

$$t_s = \frac{D_{d,0}^2 - \sqrt{D_{d,0}^4 - 9\,\frac{4k\,\mu}{(\rho_d - \rho)\,g\,f} H_d}}{k}$$

$$L_d = \begin{cases} \sqrt{4BU_0R_0}\, t_l^{\frac{1}{2}}, \text{when } t_l \le t_{inj} \\ \sqrt{4BU_0R_0}\, t_{inj}^{\frac{1}{4}} t_l^{\frac{1}{4}}, \text{when } t_l \ge t_{inj} \end{cases}$$

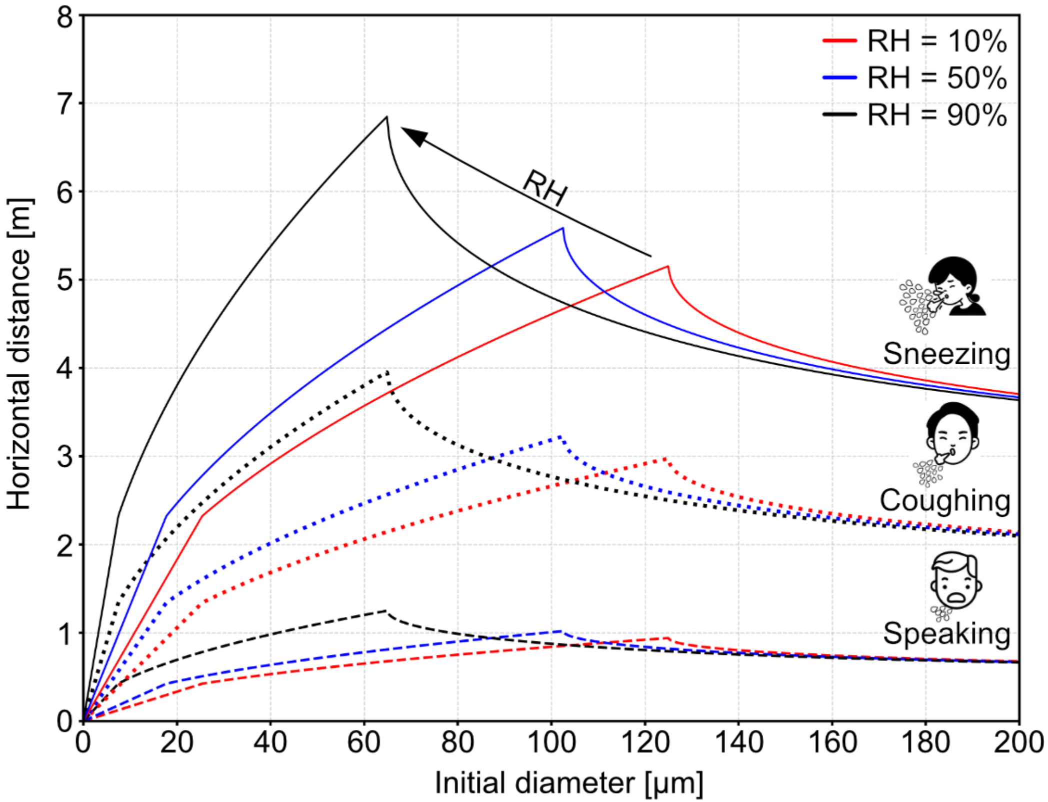
Test our model





- The present results predicted with our model are in excellent agreement with the reference data of Xie et al. (2007).

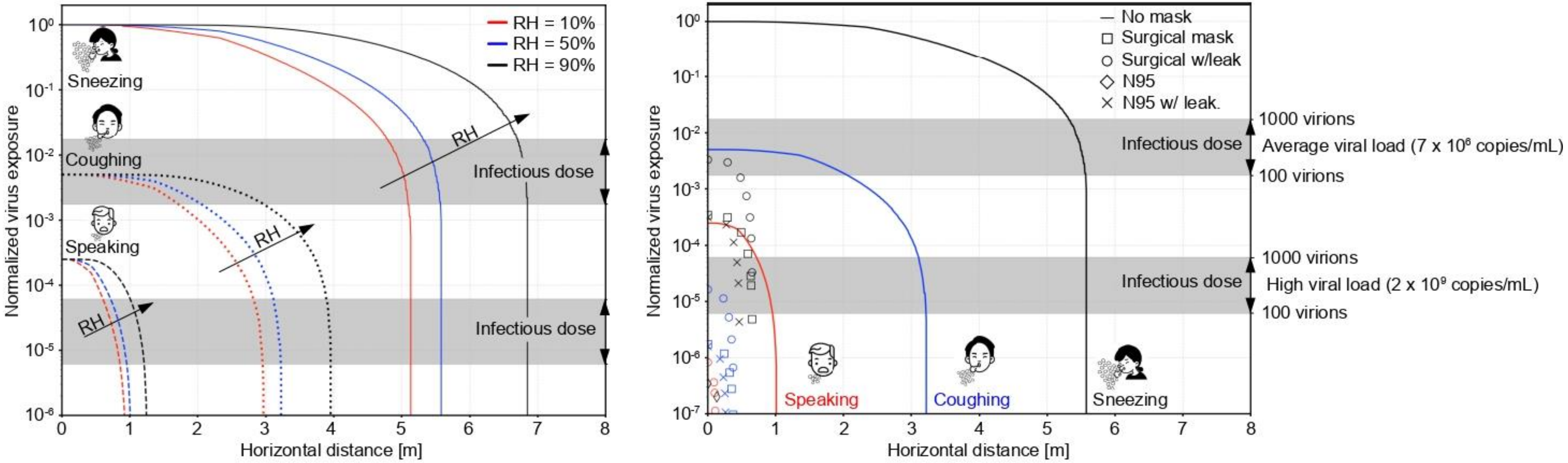
Traveling distances of drops



- ➢ Max distances:
- • 5-7 m for sneezing
- • 3-4 m for coughing
- • ~1 m speaking
- ➢ In Bourouiba's experimental analysis, "…Peak exhalation speeds *(of sneeze)* can reach up to 10-30 m/s, creating a cloud that can span approximately 7-8 m…"
- ➢ Abkarian, M. et al. reported 1~2 m distance related to speaking events.
- ✓ The model estimates for speaks and sneezes are consistent with previous experimental findings!

- *Bourouiba, L. (2016). N. Engl. J. Med., 375(8), e15.*
- *Bourouiba, L. (2020). Jama, 323(18), 1837-1838.*
- *Abkarian, M. et al. (2020). PNAS, 117(41), pp.25237-25245.*

Physical distancing & face covering



- The exposure risk is impacted by both variables, which indicates the non-existent of a universal safe distance, but more a quantitative reduction of the exposure risk with distance;
- Wearing face marks provides an excellent protection, effectively limiting the infection risk even at short physical distances, i.e. less than 1 meter.

Research Program

	1	2	3	4	5
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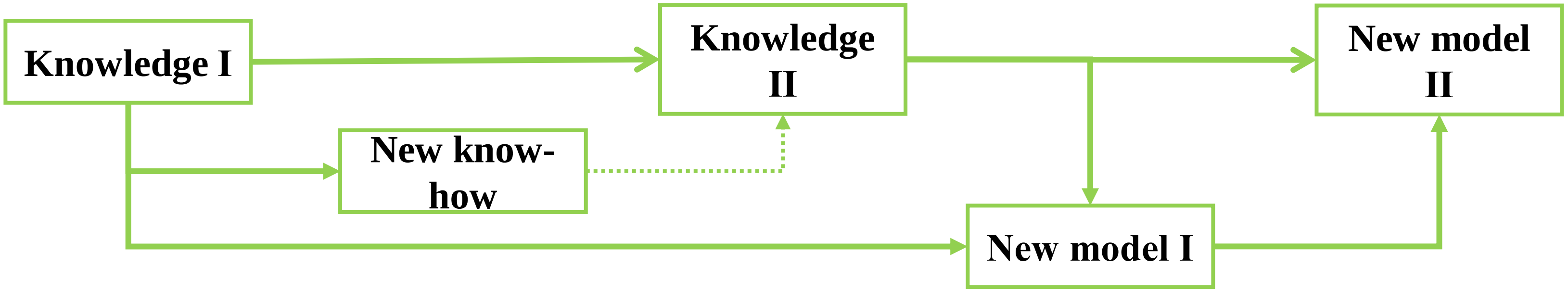
Status:	*Completed*	Completed (not shown)	*Completed*	*Completed*	*Completed*

Flow:



Final Remarks - 1/2

- ✓ We firstly showed that, in a DNS of high-Re turbulent spray, droplets form clusters surrounded by high vapor concentration; the classical evaporation model, D^2-*law*, strongly underestimate droplet evaporation time.

- ✓ We performed accurate simulations of droplet-laden turbulent puffs emitted during sneezes in a wide range of environmental conditions.

- ✓ Strong variation in droplets' evaporation or condensation in accordance with their local temperature and humidity microenvironment; and the incorrect definition of aerosols.

- ✓ Models currently used in public health guidelines grossly underestimate, by at least one order of magnitude, the actual evaporation times. Meanwhile the classical theory scaling seems to bear some universality.

Final Remarks - 2/2

- ✓ We revised the classical D^2-law by a proper estimate of the asymptotic droplet properties, which provides a superior description of droplet evaporation with respect to the classical model;

- ✓ We proposed an effective framework for respiratory droplets to assess the virus infection risk related to the direct contagion route, with which the impact of physical distancing and face-covering on limiting infection risk has been quantified considering different environmental conditions and respiratory events.

Academic outputs

Publications

- Wang, J. & Picano, F. (2021). Modeling Lagrangian droplets within a turbulent spray with the LES method. In preparation.
- Wang, J., Dalla Barba, F., Roccon, A., Sardina, G., Soldati, A., & Picano F. (2021). Modeling the direct virus exposure risk associated with respiratory events. ***J. R. Soc. Interface***, In press.
- Wang, J., Alipour, M., Soligo, G., Roccon, A., De Paoli, M., Picano, F., & Soldati, A. (2021). Short-range exposure to airborne virus transmission and current guidelines. ***Proc. Natl. Acad. Sci. U.S.A.,*** 118 (37), e2105279118.
- Dalla Barba, F., Wang, J., & Picano, F. (2021). Revisiting D2-law for the evaporation of dilute droplets. ***Phys. Fluids***, 33(5), 051701.
- Wang, J., Dalla Barba, F., & Picano, F. (2021). Direct numerical simulation of an evaporating turbulent diluted jet-spray at moderate Reynolds number. ***Int. J. Multiph. Flow***, 137, 103567.

Conferences (Oral presentation)

- 74th Annual Meeting of the APS Division of Fluid Dynamics, APS, Phoenix, Arizona, November 21-23, 2021.
- 18th Multiphase Flow Conference, HZDR, Online, November 08-12, 2021.
- EUROMECH Colloquium 621: Transport and Flexes in Dispersed Turbulent Flows, EUROMECH, Online, June 30 - July 02, 2021
- 1st BICTAM-CISM Symposium on Dispersed Multiphase Flows: From Measuring to Modeling, BICTAM-CISM, Online, March 02-05, 2021.

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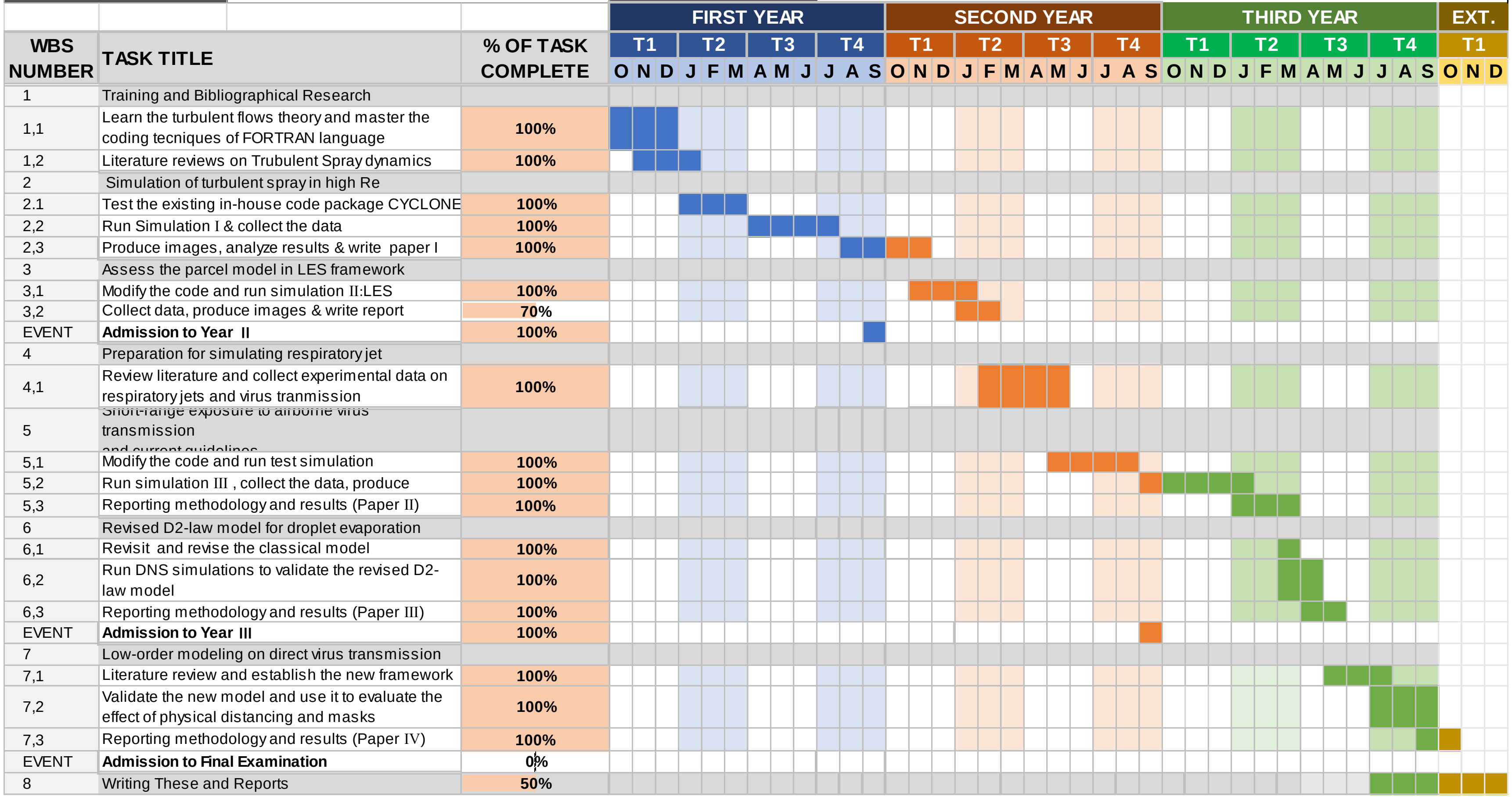
GANTT CHART

PHD STUDENT	**Jietuo Wang**	**DATE**	06/12/2021
PHD THESIS	**Simulation and modeling of turbulent spray dynamics**	**ADMISSION TO**	Final Examination



WBS NUMBER	TASK TITLE	% OF TASK COMPLETE	FIRST YEAR												SECOND YEAR												THIRD YEAR												EXT.		
			T1			T2			T3			T4			T1			T2			T3			T4			T1			T2			T3			T4			T1		
			O	N	D	J	F	M	A	M	J	J	A	S	O	N	D	J	F	M	A	M	J	J	A	S	O	N	D	J	F	M	A	M	J	J	A	S	O	N	D
1	Training and Bibliographical Research																																								
1,1	Learn the turbulent flows theory and master the coding tecniques of FORTRAN language	100%	■	■	■																																				
1,2	Literature reviews on Trubulent Spray dynamics	100%		■	■	■																																			
2	Simulation of turbulent spray in high Re																																								
2.1	Test the existing in-house code package CYCLONE	100%				■	■	■																																	
2,2	Run Simulation I & collect the data	100%							■	■	■	■																													
2,3	Produce images, analyze results & write paper I	100%											■	■	■	■																									
3	Assess the parcel model in LES framework																																								
3,1	Modify the code and run simulation II:LES	100%														■	■	■																							
3,2	Collect data, produce images & write report	70%																■	■																						
EVENT	**Admission to Year II**	100%												■																											
4	Preparation for simulating respiratory jet																																								
4,1	Review literature and collect experimental data on respiratory jets and virus tranmission	100%																	■	■	■	■																			
5	Short-range exposure to airborne virus transmission and current guidelines																																								
5,1	Modify the code and run test simulation	100%																				■	■	■	■																
5,2	Run simulation III , collect the data, produce	100%																								■	■	■	■	■											
5,3	Reporting methodology and results (Paper II)	100%																												■	■	■									
6	Revised D2-law model for droplet evaporation																																								
6,1	Revisit and revise the classical model	100%																														■									
6,2	Run DNS simulations to validate the revised D2-law model	100%																														■	■								
6,3	Reporting methodology and results (Paper III)	100%																															■	■							
EVENT	**Admission to Year III**	100%																								■															
7	Low-order modeling on direct virus transmission																																								
7,1	Literature review and establish the new framework	100%																																■	■	■					
7,2	Validate the new model and use it to evaluate the effect of physical distancing and masks	100%																																		■	■	■			
7,3	Reporting methodology and results (Paper IV)	100%																																				■	■		
EVENT	**Admission to Final Examination**	0%																																							
8	Writing These and Reports	50%																																		■	■	■	■	■	■

Thanks for the attention

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