CBE 40445

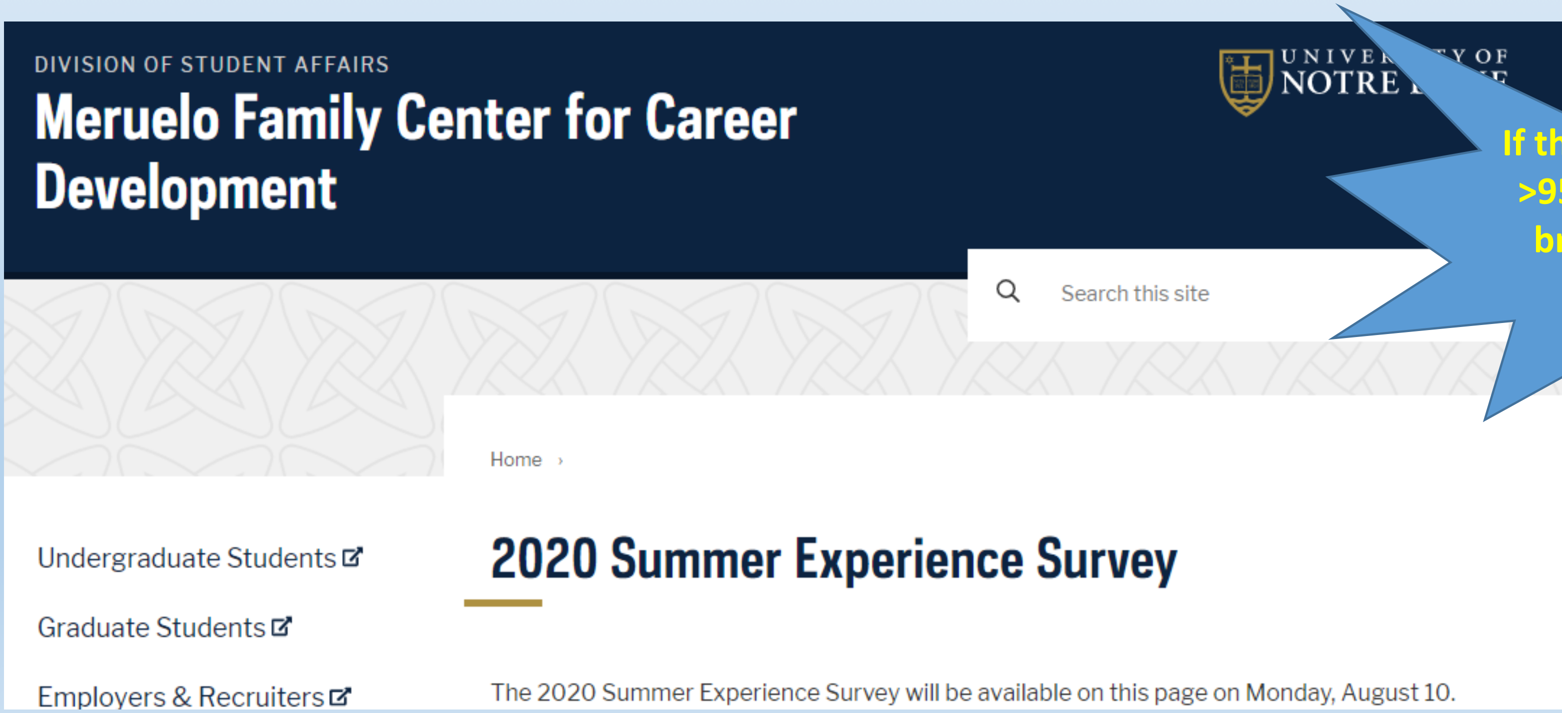
8/10/20

Review of key ideas from previous ChEg courses and how they enlighten the current epidemic

Engineering Summer Experience Survey

Please take the next 5 minutes to complete this survey on your phone or computer indicating what you did during the summer of 2020.

The Survey is on the College of Engineering Homepage: https://careerdevelopment.nd.edu/summer2020/
Login with your ND userID



If the response rate is >95%, candy will be brought in for the entire class

If you have trouble logging in, email Willerton@nd.edu and he can send you the survey via email

CBE 40455 Chemical Reaction Engineering
Fall 2020
MWF 10:25-11:15
101 Jordan and (live online)

Synopsis:

Our understanding of fluid flow, mass and heat transfer, thermodynamics and chemistry are directed toward developing and understanding procedures and processes to optimally synthesize useful quantities of commodity and specialty chemicals and products.

The topics will include fundamentals of reaction kinetics and catalysis, analysis of various reactor configurations and operating strategies and synthesis pathways for simple and complex molecules. Applications will be drawn from "classic" chemical engineering and the pharmaceutical, materials and food industries. We will also use our "rich" tool set to analyze various living systems and necessarily the COVID-19 epidemic.

Instructor:
Mark J. McCready
Offices: 257I Fitzpatrick Hall and 340 McCourtney,
email: mjm@nd.edu
There will be ~3 Zoom office hour/problem sessions. One will be on Thursday evening, others to be determined.

Teaching Assistant: ?

Textbook:
Fundamentals of Chemical Reaction Engineering, M. E. Davis, R. J. Davis (originally McGraw-Hill 2003). Now available online: https://authors.library.caltech.edu/25070/1/FundChemReaxEng.pdf
(Feel free to thank the authors for making this excellent text available for free.)

Course Grading:
Homework: 10% (1 set/week due on Fridays)
"midsession" hour exams: 40%. (9/4, **10/21 — changed from first version**)
Two final session exams 50% (9/25,11/20)

Additional Info:

It is presumed that all students will follow the: *Undergraduate Academic Code of Honor*.

Some of the "Covid" procedures may still be under development, but the three that could be of most importance:

1. Wear masks as directed. Professor Leighton and I have tested them. If they fit, they work!
2. You will need to sit at one of the seats labeled "Here". I presume you will settle into a favorite spot and as engineers, you could probably remember on Friday where you sat last Friday. But how about if someone takes on the "leadership" opportunity to remind the instructor to take "pano" shot of the classroom each day!
3. Don't cross the green line:

And to topics beyond traditional chemical engineering to develop and refine your engineering skills!

For each new use of a "fundamental topic", I'll point it out and make a point of "wallowing" in the fundamentalism!

CBE 40445
Fall 2020
Syllabus

1. Overview/review of chemical engineering fundamentals with applications to the COVID-epidemic. (2 classes)
2. Reaction equilibrium, reaction kinetics (4 classes). (D&D chapt. 1,2)
3. Chemical reactor configurations (4 classes). (D&D, chapt. 3)
   (hour test 1)
4. Modeling of catalyzed chemical reactions (3 classes) (D&D chapt. 4.)
5. Mechanistic description of heterogenous catalytic reactions (2 classes). (D&D chapt. 5)
   Internal and external transport limitations of catalytic reactions (4 classes) (D&D chapt. 6
   (end of 1/2 semester 1, "**final exam1**")

6. Nonideal flow in chemical reactors (2 classes) (D&D chapt. 8)
7. Nonisothermal reactors (3 classes) (D&D chapt. 9)
8. Other aspects of reactor design (2 classes) (D&D chapt. 10)
9. Polymerization reactions (1.5 classes).
10. Chemical vapor deposition reactions (1.5 classes).
    (**hour test 2**)
11. Fermentation and other biological reactions (4 classes)
12. Applications of reaction engineering to biofilms (3 classes)
13. Applications of reaction engineering to describe environmental processes (3 classes)
14. ("**final exam2**")

CBE 40445
Fall 2020
Course Goals

Students who complete this course should be able to:

1. Develop and appropriately apply the design equations for CSTR, Batch and Plug Flow reactors for kinetic or thermodynamic-limited reactions, under isothermal and adiabatic conditions.

2. Understand the advantages of these different reactors depending on the kinetics and production needs.

3. Understand different reaction mechanisms and correctly obtain kinetic expressions from experimental data.

4. Apply understanding of transport phenomena and thermodynamics to reacting systems to determine how the intrinsic rate can be limited by external factors.

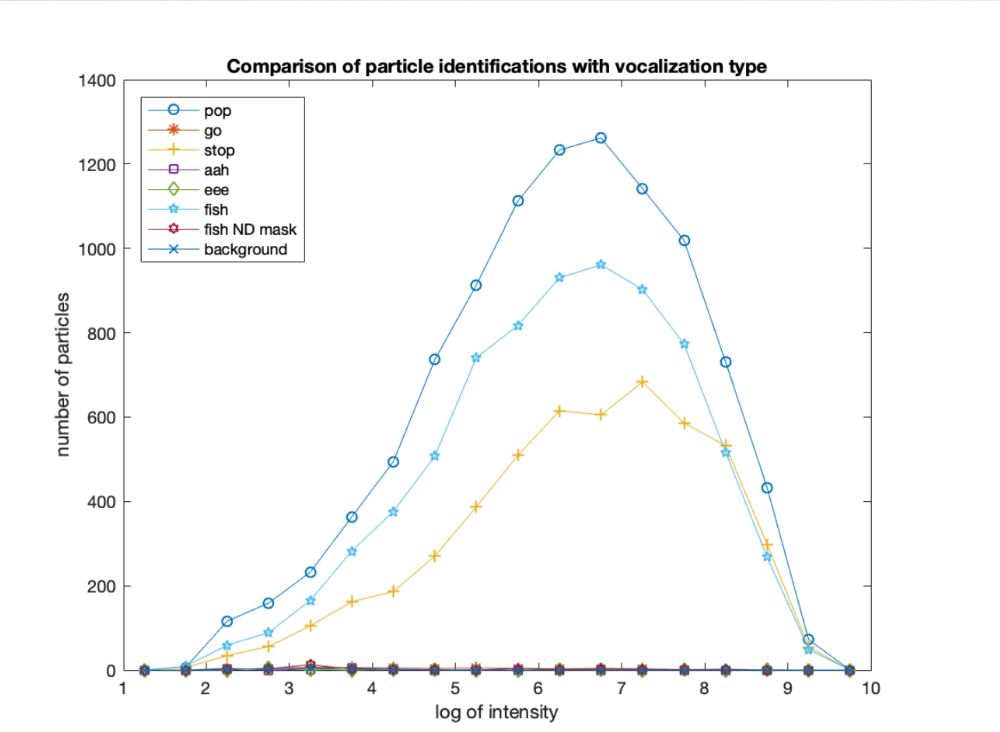
5. Understand yield, selectivity and production and how these affect reactor design and operation.

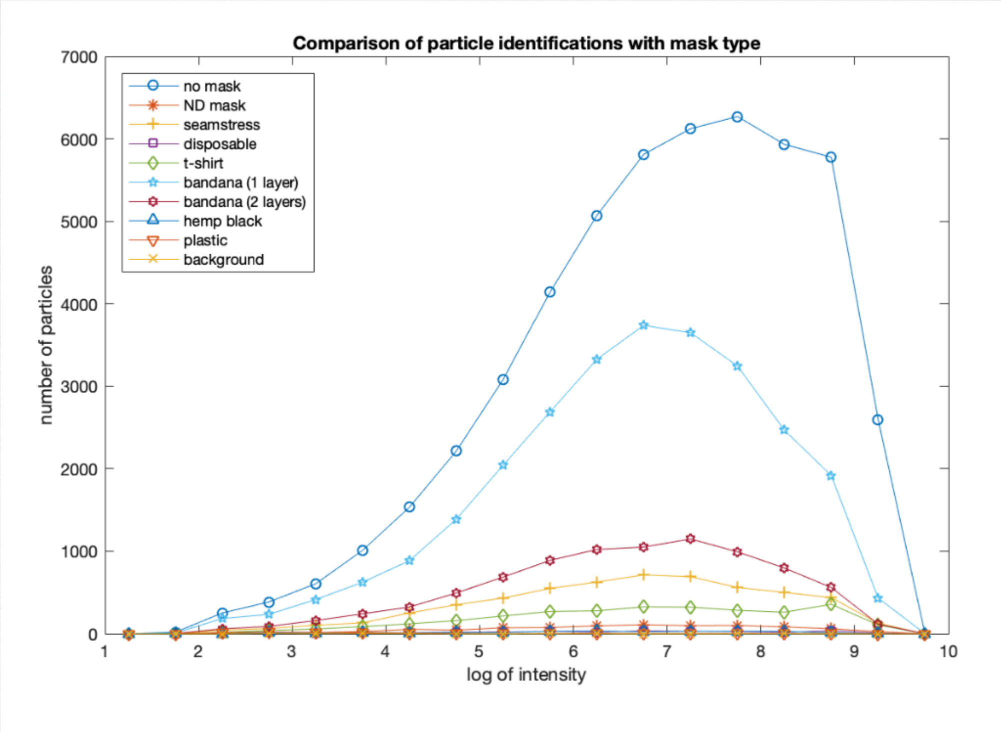
6. Understand how a chemical reactor will link with a separation train and how reactor operation may be altered to optimize the entire process.

7. Apply analysis presented in this class to biological systems and other nontraditional situations.

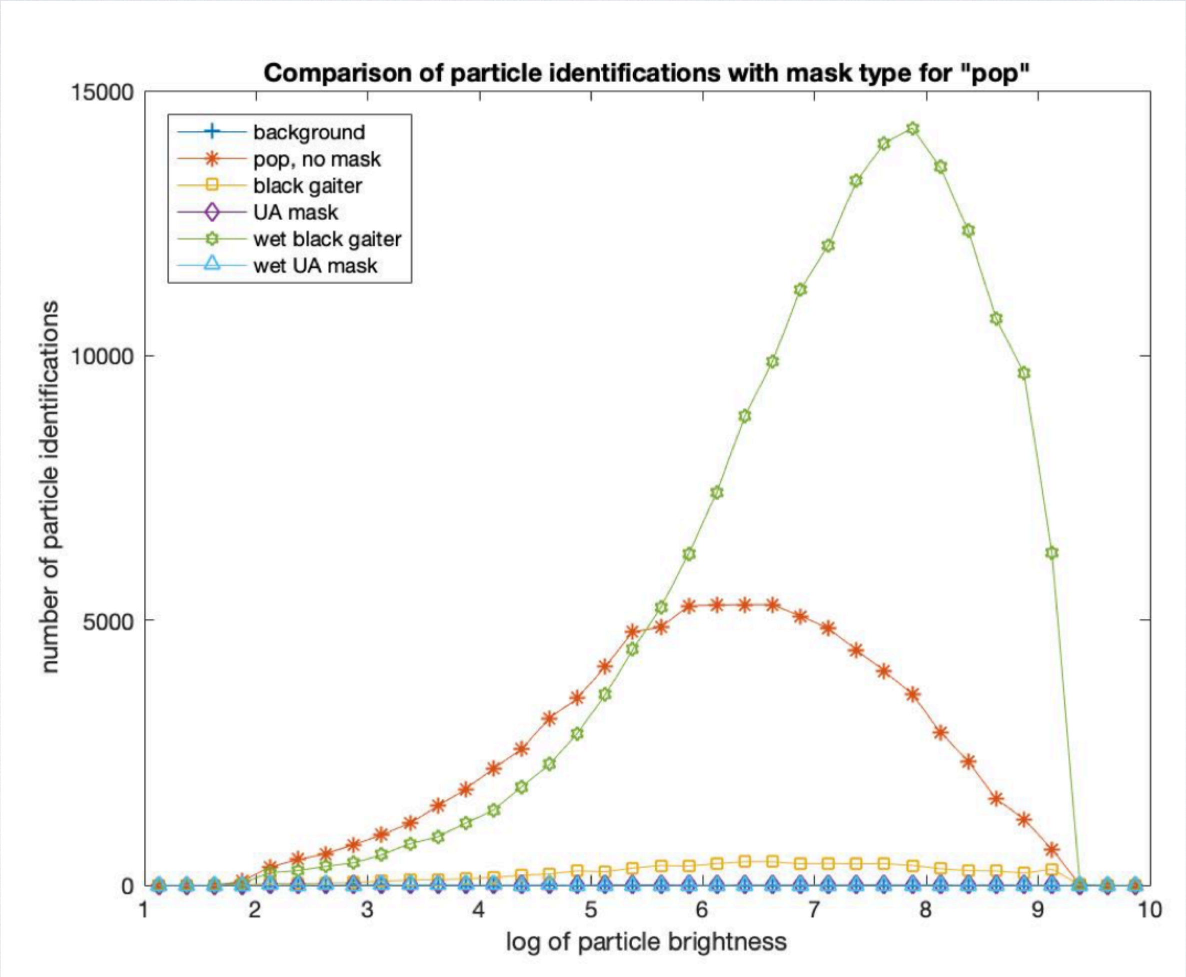
PLEASE FOLLOW THE "RULES"

- We have examined some of the relevant issues.





WET GAITERS DON'T WORK



CBE 30355/30357

- Particle emission and transmission from a sneeze?

JOURNAL OF THE ROYAL SOCIETY Interface

rsif.royalsocietypublishing.org

Research

Cite this article: Han ZY, Weng WG, Huang QY. 2013 Characterizations of particle size distribution of the droplets exhaled by sneeze. J R Soc Interface 10: 20130560.
http://dx.doi.org/10.1098/rsif.2013.0560

Received: 24 June 2013
Accepted: 21 August 2013

Subject Areas:
bioengineering, biomechanics, biophysics

Characterizations of particle size distribution of the droplets exhaled by sneeze

Z. Y. Han, W. G. Weng and Q. Y. Huang

Department of Engineering Physics, Institute of Public Safety Research, Tsinghua University, Beijing 100084, People's Republic of China

This work focuses on the size distribution of sneeze droplets exhaled immediately at mouth. Twenty healthy subjects participated in the experiment and 44 sneezes were measured by using a laser particle size analyser. Two types of distributions are observed: unimodal and bimodal. For each sneeze, the droplets exhaled at different time in the sneeze duration have the same distribution characteristics with good time stability. The volume-based size distributions of sneeze droplets can be represented by a lognormal distribution function, and the relationship between the distribution parameters and the physiological characteristics of the subjects are studied by using linear regression analysis. The geometric mean of the droplet size of all the subjects is 360.1 μm for unimodal distribution and 74.4 μm for bimodal distribution with geometric standard deviations of 1.5 and 1.7, respectively. For the two peaks of the bimodal distribution, the geometric mean (the geometric standard deviation) is 386.2 μm (1.8) for peak 1 and 72.0 μm (1.5) for peak 2. The influences of the measurement method, the limitations of the instrument, the evaporation effects of the droplets, the differences of biological dynamic mechanism and characteristics between sneeze and other respiratory activities are also discussed.

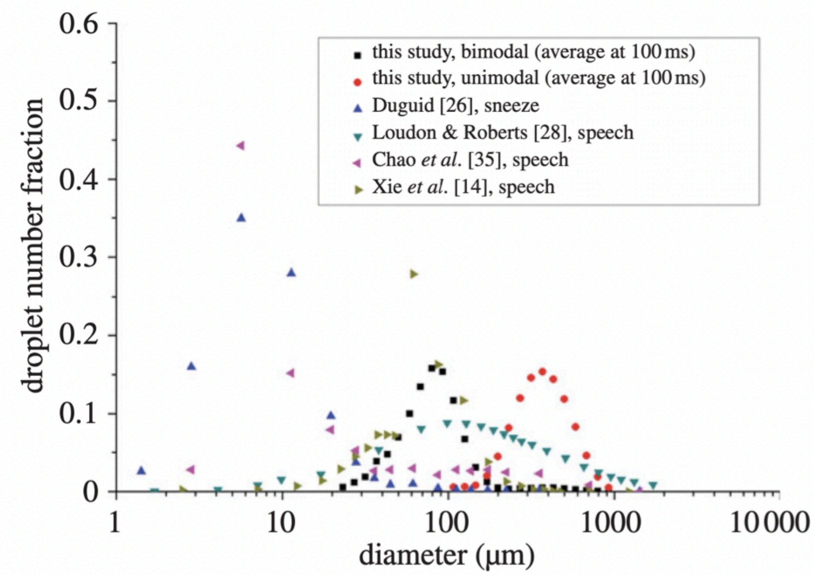


Figure 5. Comparison of the number size distribution of the droplets exhaled by sneeze and speech. (Online version in colour.)

If we want to find out how far a sneeze droplet will go, a first approximation is to use Newton's 2nd law of motion

$$\frac{d\vec{P}}{dt} = \sum_i \vec{F}_i$$

$$F_d = \frac{1}{2}\,\rho\,u^2\,c_d\,A$$

Drag coefficient

Reynolds number: $\mathrm{Re} = \frac{D_p V_p \rho}{\eta}$

drag coefficient: $C_D = \frac{8}{\pi}\frac{F_D}{\rho V_p^2 D_p^2}$

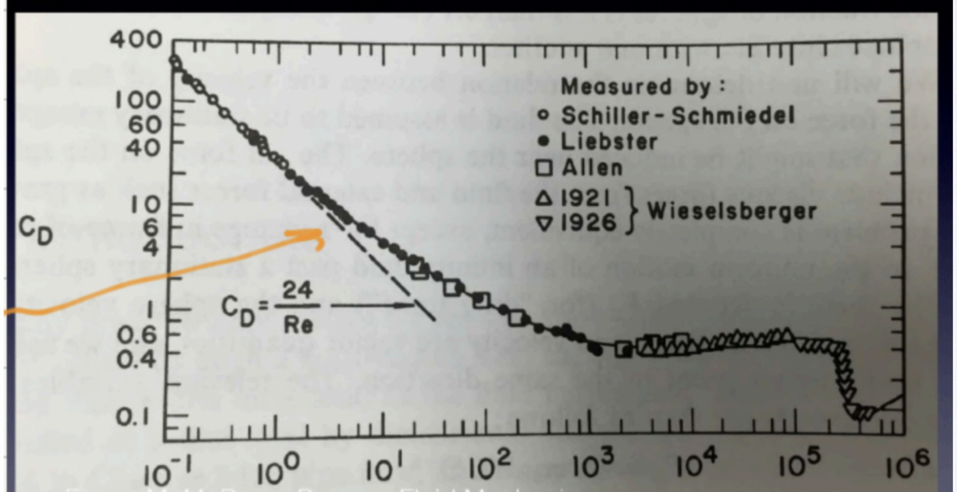
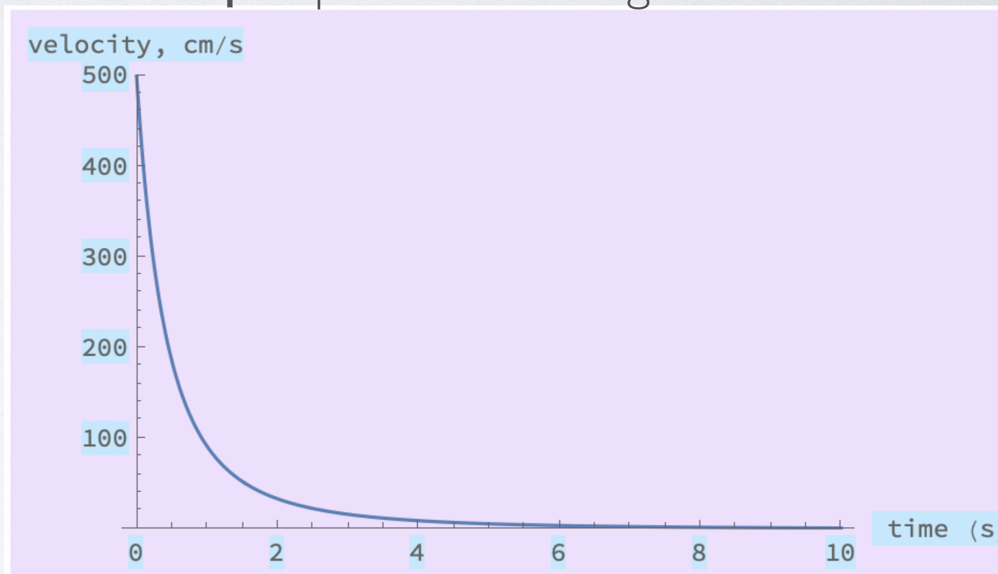


Figure 4-1. Drag coefficient as a function of Reynolds number for flow past a sphere. (Reproduced from H. Schlichting, *Boundary Layer Theory*, 6th ed., McGraw-Hill Book Company, New York, 1968, by

For a 100 μm particle starting at 5 m/s



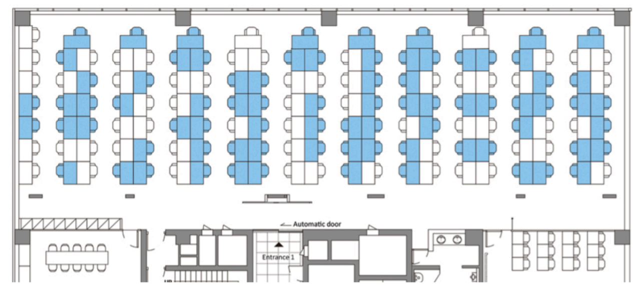
Total distance is about 3 m!

CBE 20255

- How safe are we in this room?
  - Spread of virus by aerosols is possible…
- This seemed pretty obvious from the beginning if only recently acknowledged by WHO and CDC
- Some of the particles from speaking are too small to get filtered by masks.
- You emit small particles by just breathing.

CBE 20255
Spring 2020
Final Exam
5/7/20

1. Potential for aerosol spread of SARS CoV 2 virus.



EMERGING INFECTIOUS DISEASES®

EID Journal > Volume 26 > Number 8—August 2020 > Main Article

Volume 26, Number 8—August 2020

Synopsis

Coronavirus Disease Outbreak in Call Center, South Korea

AEROSOL SPREAD

- Particles small enough to remain suspended in air are small and thus don’t carry much virus.
- All through the spring I saw the same people working at my local “essential businesses” — they were certainly encountering infected people.
- No apparent “excess” musician deaths after Mardi-Gras!

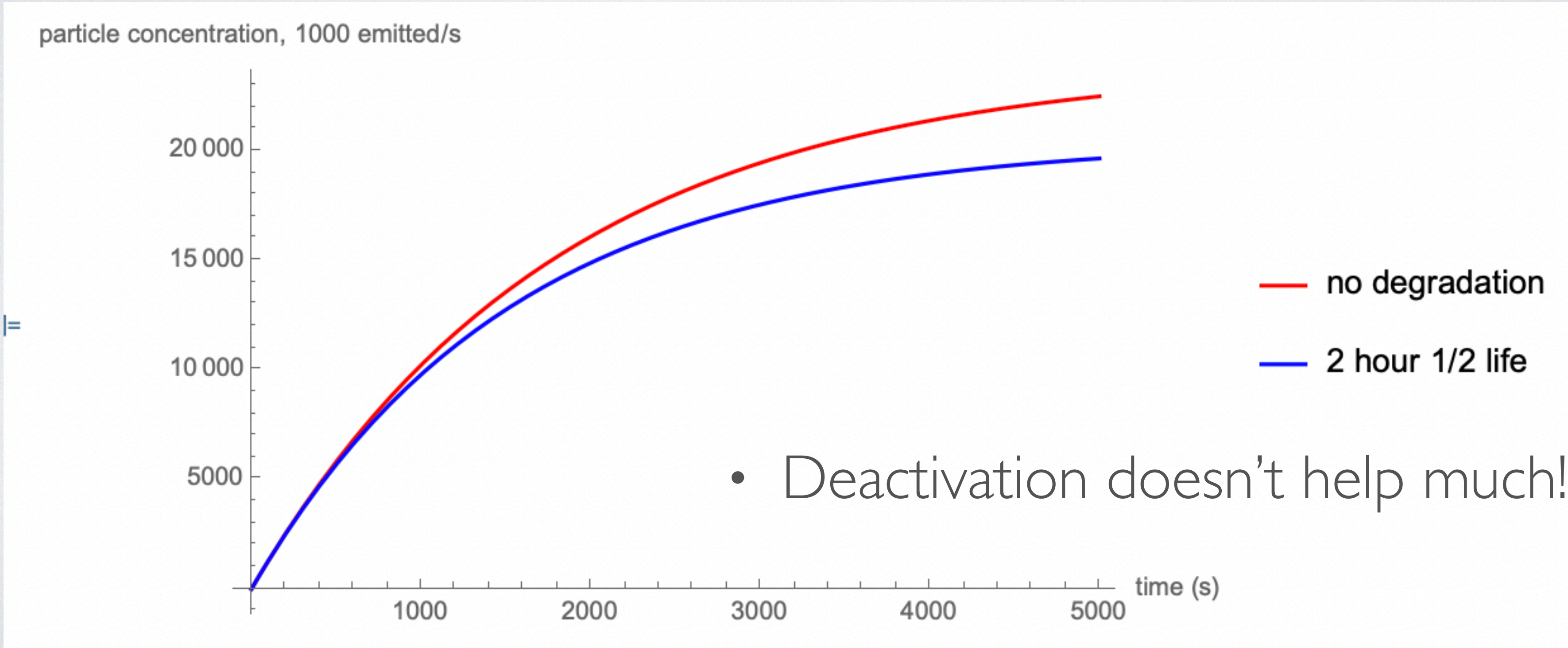
ANALYSIS OF AEROSOL SPREAD

- “Component” mass balance for “spittle” particles that (for consistency) come from speaking.
    - For a range of sizes, even if they initially fall because of gravity, they can evaporate to become aerosolized.
- ***V***— volume of room, $\boldsymbol{c}_p$(t)— particle concentration, ***q***—volumetric ventilation rate, ***S***— particle emission rate, ***k***— first order rate constant for deactivation of virus

In[•]:= $$\mathbf{eq1} = \frac{\partial(V\,\mathrm{cp}(t))}{\partial t} == -k\,V\,\mathrm{cp}(t) - q\,\mathrm{cp}(t) + S$$

SOLVE FOR INITIALLY NO VIRUS

$$\mathbf{cp}[t] = \frac{S\left(1 - e^{-t\left(k+\frac{q}{V}\right)}\right)}{k\,V + q}$$

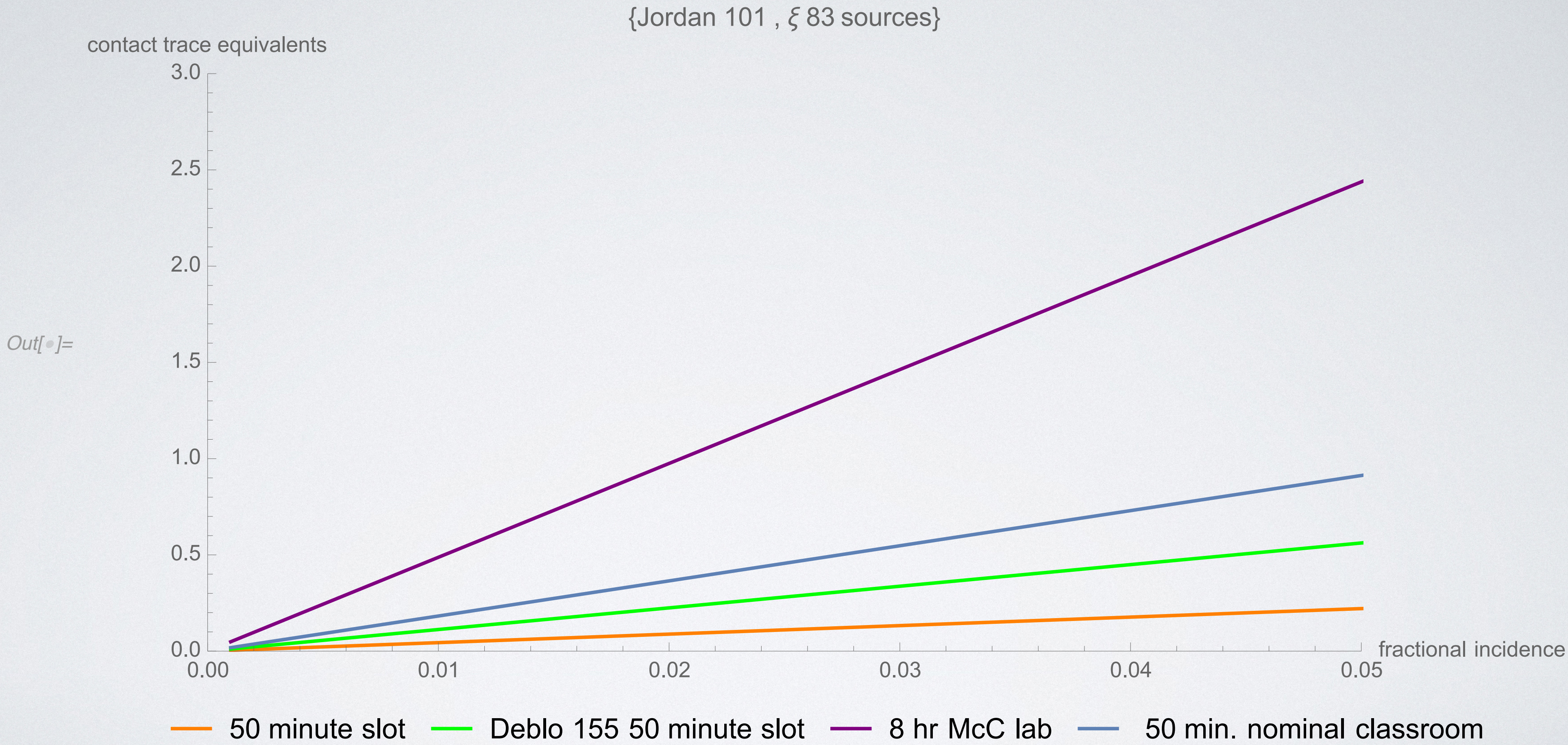


- Deactivation doesn't help much!

AEROSOL "THREAT"

- Define a "safe" dose of particles…
  - "Contact trace"… what you might get 6 feet from someone speaking for 15 minutes
    - Spherical spread of particles… you breath in a fraction of the flux
- Specify "emission" in terms of incidence of infection and numbers of people present
- Ventilation by size of room.

HOW SAFE ARE WE NOW?



CBE 30367, 30356

- Why does humidity matter?
  - The virus is present in saliva, so "humid air" doesn't degrade it faster.
- There is a range of particles emitted by speaking that evaporate before hitting the ground. Since these are the largest sized particles that become aerosolized, these could be the biggest threat.
  - 100 μm, v = 30 cm/s, 50 μm, v = 7.5 cm/s, 20 μm, v = 1.2 cm/s.
- How much faster would an emitted particle evaporate in rooms with different relative humidity and temperature? (HW problem for you!)

PARTICLE EVAPORATION

This competition has been extensively studied, and a useful summary for clean water drops and typical room air conditions is provided by Barrow and Pope (J Ap Energy, 2006, doi:10.1016/j.apenergy.2006.09.007):

Table 1
Evaporation time and distance travelled by a droplet in free-fall

Droplet diameter (μm)	Time (s)	Distance (m)
25	0.66	0.006
50	2.54	0.097
75	5.39	0.457
100	9.00	1.337
125	13.17	3.0
150	17.84	5.79
200	28.00	15.70

Terminal temperature = 291.1 K.
Initial temperature = 288.5 K.
Environment temperature = 301 K.
Environment relative humidity = 40%.

EYE PROTECTION?

THE LANCET

Access provided by University of Notre Dame

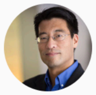
ARTICLES | VOLUME 395, ISSUE 10242, P1973-1987, JUNE 27, 2020

Physical distancing, face masks, and eye protection to prevent person-to-person transmission of SARS-CoV-2 and COVID-19: a systematic review and meta-analysis

Derek K Chu, MD • Prof Elie A Akl, MD • Stephanie Duda, MSc • Karla Solo, MSc • Sally Yaacoub, MPH • Prof Holger J Schünemann, MD • et al. Show all authors • Show footnotes

EDITORS' PICK | 34,391 views | Jul 30, 2020, 02:19am EDT

Did Dr. Fauci Recommend Wearing Eye Shields, Goggles For Covid-19 Coronavirus?



Bruce Y. Lee Senior Contributor

Healthcare

I am a writer, journalist, professor, systems modeler, computational and digital health expert, avocado-eater, and entrepreneur, not always in that order.

STOKES-EINSTEIN

- Diffusivity of particles and flux to eyes.
  - For "small particles" Re<<1, Stokes law will give drag as long as the "fluid" can be considered a continuum

For .5 μm particles

```
In[∘]:= % /. {T → 298, k → 1.38×10^-16, μ → .01/55, R → .00005}
Out[∘]= 2.39987×10^-7
```

"Boundary layer"

```
In[∘]:= δ = .2 cm
Out[∘]= 0.2 cm

In[∘]:= area = 4 cm^2
Out[∘]= 4 cm^2

In[∘]:= flux = dd / δ area
Out[∘]= 4.×10^-6 cm^3 / s
```

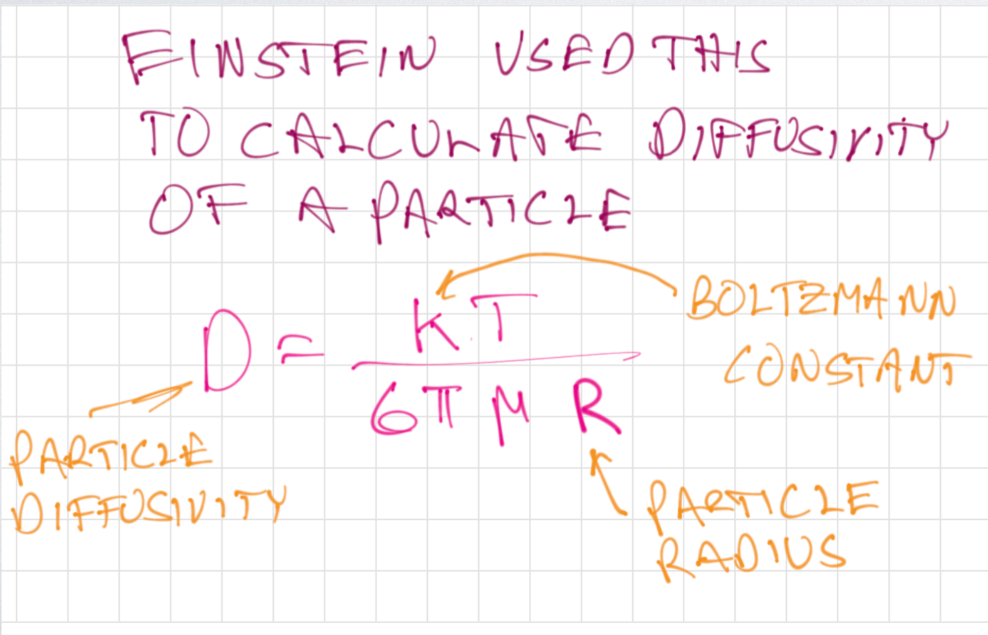
Breath input of virus

We pick 10 l/minute

```
In[∘]:= 10 l / min /. {l → 1000 cm^3, min → 60. s}
Out[∘]= 166.667 cm^3 / s
```

Ratio of eyes compared to breath!

```
In[∘]:= %6 / %7
Out[∘]= 2.4×10^-8
```



HOW DO PARTICLES GET IN?

2 *T.C. Carvalho et al. / International Jou*

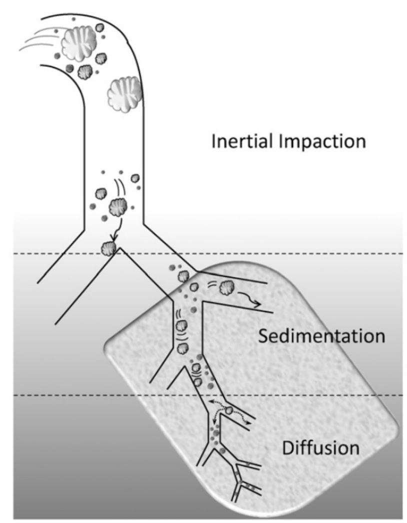


Fig. 1. Schematic diagram representing particle deposition in the lungs according to different mechanisms related to particle size: inertial impaction, sedimentation and diffusion. The diagram presents the smaller particles depositing in the lower airways as opposed to the larger airways. The GI tract is omitted in this diagram.

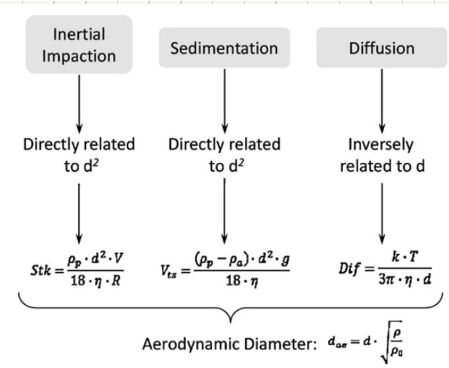


Fig. 2. The influence of particle size on deposition. *d*: particle diameter; *Stk*: Stokes number; ρ_p: particle density; *V*: air velocity; η: air viscosity; *R*: airway radius; V_{ts}: terminal settling velocity; ρ_a: air density; *g*: gravitational acceleration; *Dif*: diffusion coefficient; *k*: Boltzmann's constant; *T*: absolute temperature; d_{ae}: aerodynamic diameter; ρ_0: unity density.

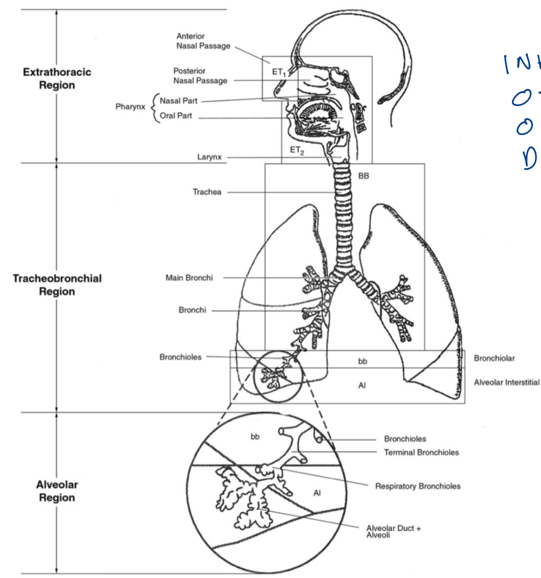


Fig. 1. Illustration of the major anatomical regions of the human respiratory tract (ICRP, 1994). *Abbreviations*: ET_1: anterior nasal passages; ET_2: posterior nasal passages, naso-oropharynx, and larynx; BB: bronchial region, including trachea and bronchi; bb: bronchiolar region consisting of bronchioles and terminal bronchioles; AI: alveolar-interstitial region, consisting of respiratory bronchioles, and alveolar ducts and sacs surrounded by alveoli.

INHALATION OF DUST... OR AEROSOL DRUG DELIVERY

TORTUOUS PATH TO SMALL PASSAGES

PARTICLES STICK TO WALL: CLEARED BY CILIA

LONG PATH: ONLY ~ LAST 5 BRANCHES ABSORB

COULD BREATH BACK OUT

ONLY A "NARROW" SIZE RANGE OF PARTICLES WILL BE DELIVERED TO INSIDE SURFACE OF LUNGS...

PAEDIATRIC RESPIRATORY REVIEWS (2003) **4**, 135–142
doi: 10.1016/S1526-0542(03)00032-0
Available online at www.sciencedirect.com
SCIENCE @ DIRECT®
Paediatric Respiratory Reviews

SERIES: DIFFICULT ASTHMA

Role of inhaler competence and contrivance in "difficult asthma"

Mark L. Everard

Department of Respiratory Medicine, Sheffield Children's Hospital, Western Bank, Sheffield S10 2TH, UK

KEYWORDS
aerosols; asthma; regime adherence; device compliance; competence; contrivance

Summary Failure to deliver drug effectively to the lungs is a common cause of referrals with "difficult asthma". This may be due to poor regime compliance or poor device compliance (lack of competence and/or contrivance). The former is the more difficult to address. The latter can be addressed providing the healthcare professional is aware of the principles underlying aerosol delivery and aspects of patient behaviour.

Unlike the gastrointestinal tract, the airways have evolved to exclude foreign material. A narrow window of opportunity exists with particles in the size range 1–7 μm having a relatively high probability of depositing within the airways once inhaled. Current delivery systems are able to generate particles in this size range but they all have associated problems that may significantly impair the effectiveness of drug delivery to the lungs.

INTRODUCTION

When faced with a patient with "difficult asthma", the following possibilities need to be carefully considered and addressed in detail before considering the less likely explanation that the patient needs the dose of medication increasing further.

- The patient does not have asthma (e.g. bronchiectasis, endobronchial infection, whooping cough, "post-viral cough" tracheomalacia, etc.).
- The patient has asthma together with a respiratory problem that is not being addressed.
- The patient is failing to deliver drugs to the lungs due to lack of compliance, lack of competence or contrivance (the 3Cs).

If a patient continues to experience significant symptoms having effectively addressed all these possibilities, it is then possible that they may have a form of the very rare "steroid resistant asthma" discussed elsewhere in this issue.

DOES THE PATIENT HAVE ASTHMA?

A diagnosis of asthma can only be made when a clear and dramatic response to asthma medication is demonstrated. This may be evidence of "reversibility", that is an increase of >12% in FEV_1 in response to inhaled β_2-agonists (in those who can perform lung function tests reliably), or, more

!!

Correspondence to: M. L. Everard. Tel.: +44-114-271-7400; Fax: +44-114-273-0522; E-mail: meverard@sch.nhs.uk

1526–0542/03/$ – see front matter

CHEM 10112, CBE 20255, CBE 40445

- Even if "*k*" was not large enough to make a difference in a classroom, how does temperature affect the rate of deactivation in other situations?

Microbes Environ. Vol. 30, No. 2, 140-144, 2015
https://www.jstage.jst.go.jp/browse/jsme2 doi:10.1264/jsme2.ME14145

MICROBES AND ENVIRONMENTS

Survival of Enveloped and Non-Enveloped Viruses on Inanimate Surfaces

SWAN FIRQUET[1], SOPHIE BEAUJARD[1], PIERRE-EMMANUEL LOBERT[1], FAMARA SANÉ[1], DELPHINE CALOONE[1], DANIEL IZARD[1,2], and DIDIER HOBER[1]*

[1]Université Lille 2, Faculté de Médecine, CHRU Lille, Laboratoire de Virologie EA3610, Lille 59037, France; and
[2]CHRU Lille Laboratoire de Bactériologie, Lille 59037, France

(Received October 9, 2014—Accepted January 13, 2015—Published online April 3, 2015)

1/2 life about 2 days

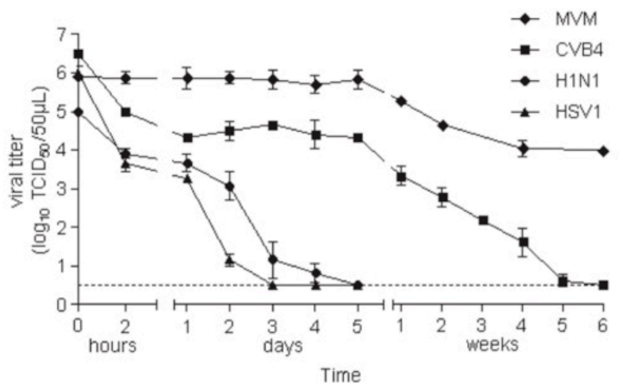


Fig. 1. Virucidal effect of drying on viruses applied to Petri dish lids. Fifty microliters of each culture supernatant fluid containing H1N1, CVB4, HSV-1, or MVM was applied to Petri dish lids in quadruplicate. They were dried under the air flow of a biosafety cabinet at room temperature from 2 h to 6 weeks. Thereafter, dried inocula were recovered using 1 mL of titer media and the infectious titers were determined and expressed as $\log_{10}$. The results are the mean ± SD of four independent experiments. The dashed line represents the detection limit of the test.

A second set of relevant data are available from:

Available online at www.sciencedirect.com
Journal of Hospital Infection
journal homepage: www.elsevier.com/locate/jhin
ELSEVIER
Healthcare Infection Society

Review

Persistence of coronaviruses on inanimate surfaces and their inactivation with biocidal agents

G. Kampf [a,*], D. Todt [b], S. Pfaender [b], E. Steinmann [b]

[a] University Medicine Greifswald, Institute for Hygiene and Environmental Medicine, Ferdinand-Sauerbruch-Straße, 17475 Greifswald, Germany
[b] Department of Molecular and Medical Virology, Ruhr University Bochum, Universitätsstrasse 50, 44801 Bochum, Germany

$$k = A\exp\left(-\frac{E_a}{RT}\right)$$

$$E_a = 120{,}000\ \frac{J}{MOLE}$$

What would you expect the half-life of the *SARS-CoV-2* (or *H1N1*) virus be at 37C?

$t = .14$ DAYS

$= 3.4$ hr.

Table I
Persistence of coronaviruses on different types of inanimate surfaces

Type of surface	Virus	Strain / isolate	Inoculum (viral titer)	Temperature	Persistence	Reference
Steel	MERS-CoV	Isolate HCoV-EMC/2012	10^5	20°C	48 h	[21]
				30°C	8–24 h	
	TGEV	Unknown	10^6	4°C	≥ 28 d	[22]
				20°C	3–28 d	
				40°C	4–96 h	
	MHV	Unknown	10^6	4°C	≥ 28 d	[22]
				20°C	4–28 d	
				40°C	4–96 h	
	HCoV	Strain 229E	10^3	21°C	5 d	[23]
Aluminium	HCoV	Strains 229E and OC43	5×10^3	21°C	2–8 h	[24]
Metal	SARS-CoV	Strain P9	10^5	RT	5 d	[25]
Wood	SARS-CoV	Strain P9	10^5	RT	4 d	[25]
Paper	SARS-CoV	Strain P9	10^5	RT	4–5 d	[25]
	SARS-CoV	Strain GVU6109	10^6	RT	24 h	[26]
			10^5		3 h	
			10^4		< 5 min	
Glass	SARS-CoV	Strain P9	10^5	RT	4 d	[25]
	HCoV	Strain 229E	10^3	21°C	5 d	[23]
Plastic	SARS-CoV	Strain HKU39849	10^5	22°-25°C	≤ 5 d	[27]
	MERS-CoV	Isolate HCoV-EMC/2012	10^5	20°C	48 h	[21]
				30°C	8–24 h	
	SARS-CoV	Strain P9	10^5	RT	4 d	[25]
	SARS-CoV	Strain FFM1	10^7	RT	6–9 d	[28]
	HCoV	Strain 229E	10^7	RT	2–6 d	[28]
PVC	HCoV	Strain 229E	10^3	21°C	5 d	[23]
Silicon rubber	HCoV	Strain 229E	10^3	21°C	5 d	[23]
Surgical glove (latex)	HCoV	Strains 229E and OC43	5×10^3	21°C	≤ 8 h	[24]
Disposable gown	SARS-CoV	Strain GVU6109	10^6	RT	2 d	[26]
			10^5		24 h	
			10^4		1 h	
Ceramic	HCoV	Strain 229E	10^3	21°C	5 d	[23]
Teflon	HCoV	Strain 229E	10^3	21°C	5 d	[23]

MERS = Middle East Respiratory Syndrome; HCoV = human coronavirus; TGEV = transmissible gastroenteritis virus; MHV = mouse hepatitis virus; SARS = Severe Acute Respiratory Syndrome; RT = room temperature.

CBE 20255, 40455

- How to model the disease spread?

- The standard method is the SIR model…

S = S(t)	is the number of *susceptible* individuals,
I = I(t)	is the number of *infected* individuals, and
R = R(t)	is the number of *recovered* individuals.

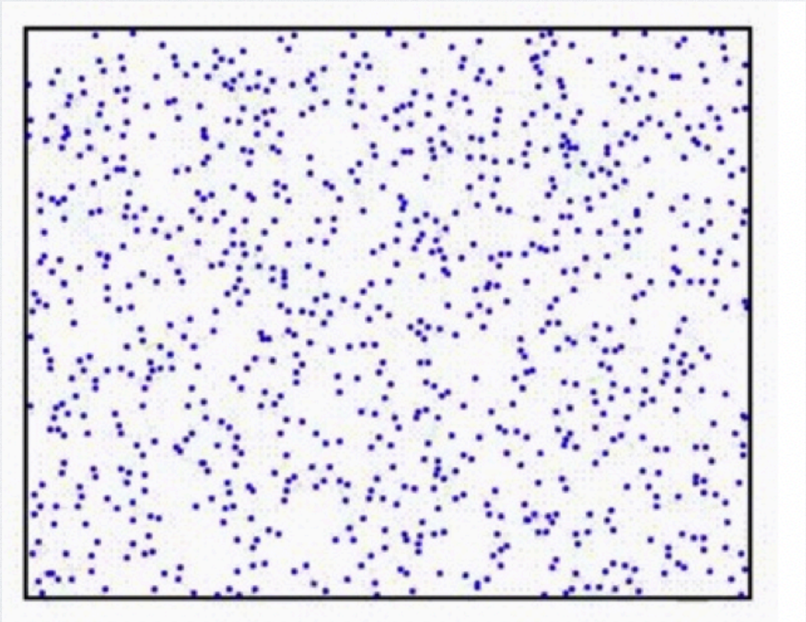
$$\frac{di}{dt} = b\, s(t)\, i(t) - k\, i(t)$$

$R_0 = b/k$ — this changes during infection, but does one location tell anything about another location?

Why was NYC so bad?

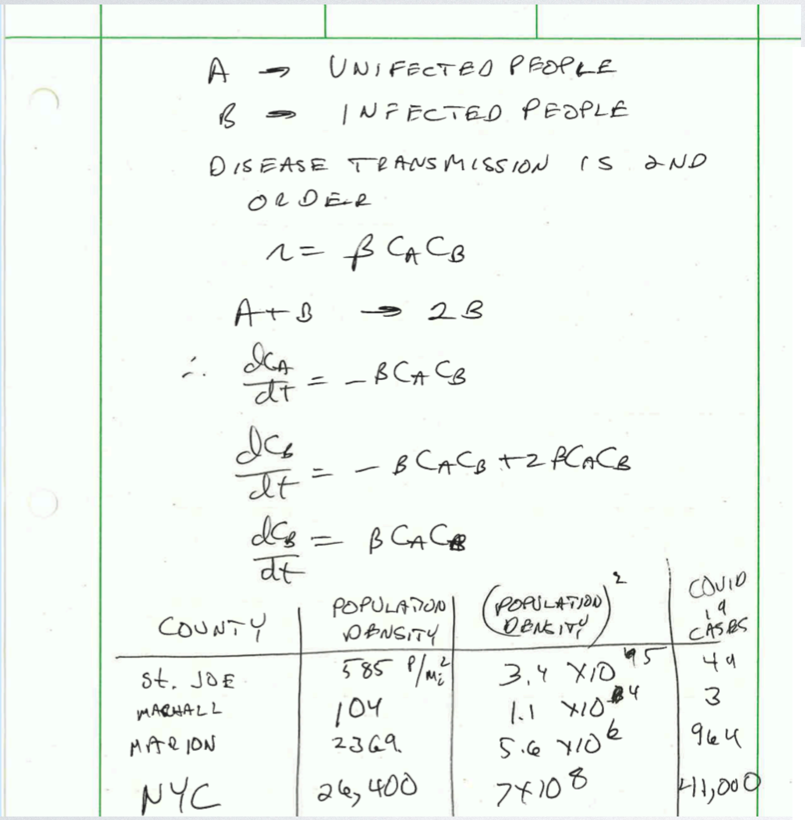
BUT WE KNOW THAT SPREAD REQUIRES A CLOSE INTERACTION!

- Hence instead of numbers of people, population density should be used.



Snapshot of ideal gas

DATA FROM MARCH 31



A → UNIFECTED PEOPLE

B → INFECTED PEOPLE

DISEASE TRANSMISSION IS 2ND ORDER

$r = \beta C_A C_B$

$A + B \rightarrow 2B$

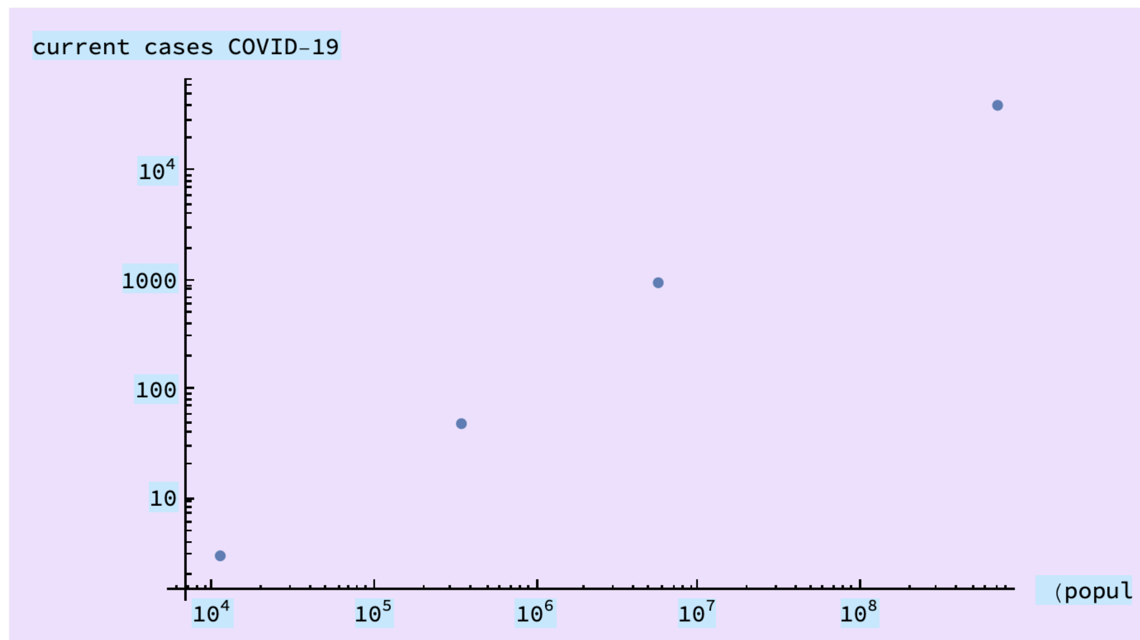
$\therefore \frac{dC_A}{dt} = -\beta C_A C_B$

$\frac{dC_B}{dt} = -\beta C_A C_B + 2\beta C_A C_B$

$\frac{dC_B}{dt} = \beta C_A C_B$

COUNTY	POPULATION DENSITY	$(\text{POPULATION DENSITY})^2$	COVID 19 CASES
St. JOE	585 P/mi^2	3.4×10^5	44
MARSHALL	104	1.1×10^4	3
MARION	2369	5.6×10^6	964
NYC	26,400	7×10^8	41,000

```
ListLogLogPlot[data,
 AxesLabel → {" (population/mi^2)^2", "current cases COVID-19"}]
```

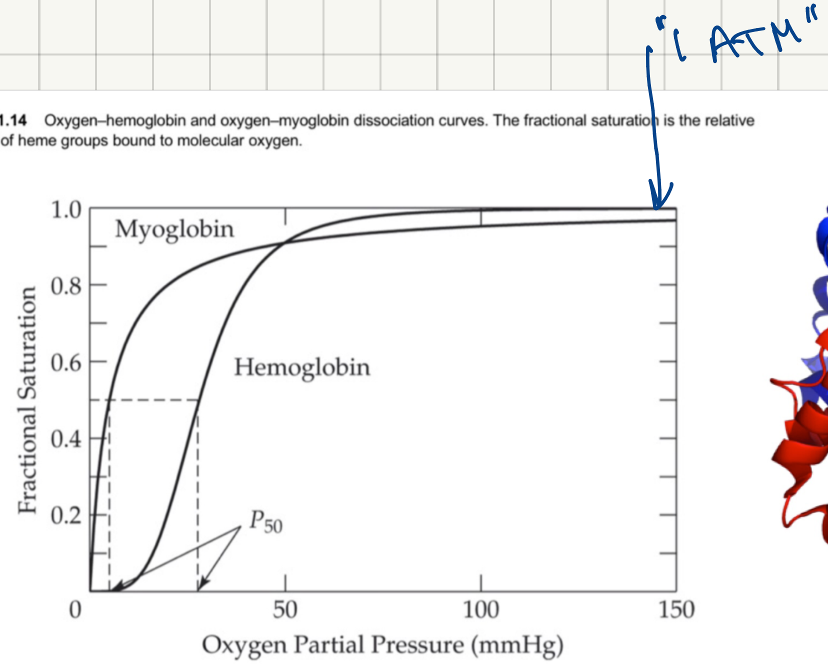


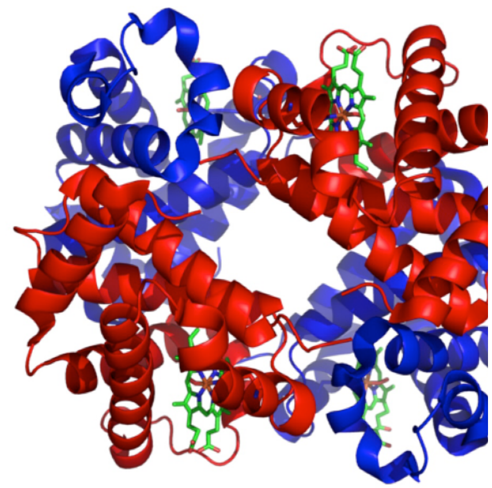
CONCLUSION FROM THIS…

- Rate constant just depends on efficiency of transmission
- Possibility of overwhelming local healthcare would only occur in the most densely populated regions.
  - … South Bend was not a few weeks behind New York, the rate of case increase was 45 times slower!

LOW BLOOD OXYGEN LEVELS

Figure 1.14 Oxygen–hemoglobin and oxygen–myoglobin dissociation curves. The fractional saturation is the relative amount of heme groups bound to molecular oxygen.





PEARSON *Transport Phenomena in Biological Systems*, Second Edition
George A. Truskey, Fan Yuan, and David F. Katz

$$C_{O_2} = H_{O_2}P_{O_2}(1 - \mathrm{Hct}) + \left(4C_{Hb}\overline{S} + H_{Hb}P_{O_2}\right)\mathrm{Hct},$$