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Influence of particle clustering on the decay rate of a passive scalar

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Outline

- Introduction and goal
- Theory
- Study setup
- Results

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Need for a model for turbulent heterogeneous combustion

— a wide range of models exist for flow turbulence itself (k-ϵ,RSM,mixing length etc.)

— a wide range of models exist for homogeneous combustion (EDC,PDF, BML)

— for liquids: spray break up, heat transfer, evaporation $\Rightarrow$ homogeneous combustion

— no model of heterogeneous combustion that takes into account flow turbulence

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We would like to change that

Simple heterogeneous reaction model: Passive scalar

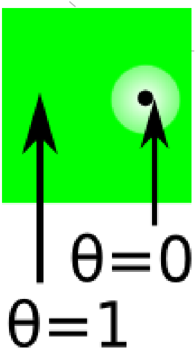
Surface specific consumption rate of species θ (e.g. oxygen) is governed by

$$\dot{n} = -\lambda X_s C_g \qquad (1)$$

the diffusion to the particle is governed by

$$\dot{n} = -k(X_\infty - X_s) \qquad (2)$$

with $k = \frac{C_g D \mathrm{Sh}}{2r_p}$ and $\mathrm{Sh} = 2$, assuming quiescent flow around particle



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Reaction model, continued

(1) $\dot{n} = -\lambda X_s C_g$
(2) $\dot{n} = -k(X_\infty - X_s)$

Equations 1 and 2 combined give

$$X_s = \frac{kX_\infty}{C_g + \lambda k} \tag{3}$$

The consumption rate can be expressed as:

$$\dot{n} = -\tilde{\lambda} X_\infty C_g \tag{4}$$

for

$$\tilde{\lambda} = \frac{\lambda k}{\lambda C_g + k}. \tag{5}$$

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Decay rate for homogeneous particle distribution

The molar fraction of θ has the behaviour

$$\frac{d\bar{X}_\infty}{dt} = -n_p \tilde{\lambda} \bar{X}_\infty \bar{A}_p \tag{6}$$

which has the solution

$$\bar{X}_\infty(t) = X_{\infty,0} e^{-\alpha_p t} \tag{7}$$

with

$$\alpha_p = n_p \tilde{\lambda} \bar{A}_p \tag{8}$$

This α_p is what we're after.
Important for later: $\frac{1}{\alpha_p} = \tau_c$

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The Damköhler number

In our system, the Damköhler number (ratio of turbulent to chemical time scales τ_p to τ_c) can be defined as

$$\mathrm{Da} = \frac{\tau_{flow}}{\tau_c} = \frac{\tau_p}{\tau_c} \tag{9}$$

where we set the τ_{flow} as the timescale of the eddies responsible for particle clustering. If $\mathrm{St}_{part} = 1$, we can say $\tau_{flow} \approx \tau_{particle}$.

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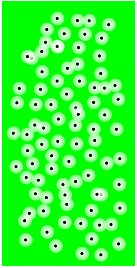
Small Damköhler number and decay rate

For small Damköhler numbers it is possible to reorganize $\mathrm{Da} = \frac{\tau_{flow}}{\tau_c} = \alpha_p \tau_p$ to obtain:

$$\alpha_p = \frac{\mathrm{Da}}{\tau_p} \qquad (10)$$

⇒small Damköhler ⇒ decay rate α_p scales with Damköhler number.



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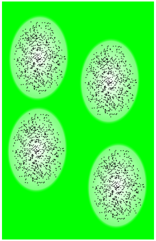
Large Damköhler number and decay rate

Large Damköhler numbers $\Rightarrow$ clusters with many particles $\Rightarrow$ "internal" θ is consumed very fast and the decay rate becomes:

$$\alpha_c = n_c \tilde{\lambda}_c \overline{A}_c \quad (11)$$



$n_c = \left(\frac{L_x}{A_1 \ell}\right)^3 \Rightarrow$ superparticle number density

$\ell = (\tau_p u_{rms})^{3/2} \sqrt{k_f} \Rightarrow$ size of cluster-creating eddies.

$A_1 \approx 9 \ldots 11 \Rightarrow$ fitting parameter to account for the non-sphericity of the superparticles.

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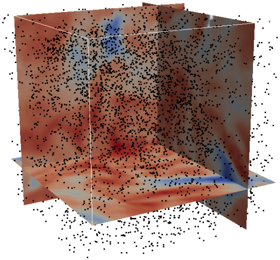
Study setup

- Eulerian-Lagrangian approach with point-particle representation
- $d_{particle} = 0.1 - 0.2\Delta x$
- $n_{particle} = 50k - 1.25M$
- prescribed forcing
- the passive scalar θ is only converted on the particle surface
- isothermal flow
- Stokes drag



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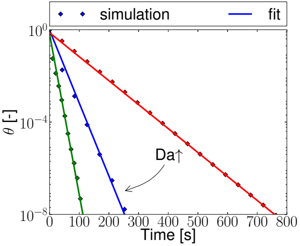
Study setup,continued

- different Stokes numbers and Damköhler numbers are studied
- simulations are run until the flow reaches statistically steady state
- then charged with $\theta = 1$, then run until the volume averaged θ drops below 1×10^{-5}
- an α_{fit} is then computed to quantify the decay rate



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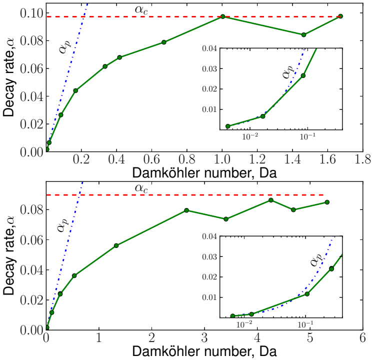
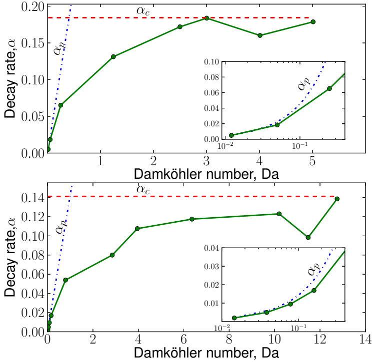
Study results





α over Da, D=1 $\times$ 10^{-3}m^2/s,
St = 0.33($\uparrow$) and 1($\downarrow$)

α over Da, D=3 $\times$ 10^{-3}m^2/s,
St = 0.33($\uparrow$) and 1($\downarrow$)

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Conclusions

- at low Damköhler numbers the decay rate *scales directly with the Damköhler number*
- for high Damköhler numbers the decay rate is limited by flow conditions and *independent of the Damköhler number*
- this effect has to be accounted for in turbulence models that don't incorporate clustering (RANS, Subgrid of LES)

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End

Thank you for your attention! Questions?

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norway grants

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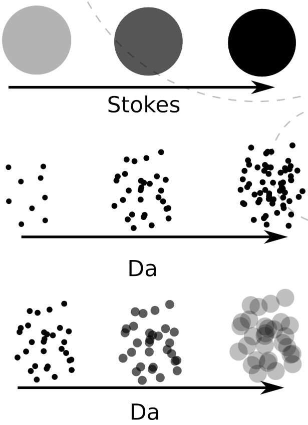
Parameters studied

- Two passive scalar diffusivities: $1 \times 10^{-3} \mathrm{m}^2/\mathrm{s}$ and $3 \times 10^{-3} \mathrm{m}^2/\mathrm{s}$
- Two different Stokes numbers: 0.33 and 1 (via change in particle density)
- Variation of Damköhler number over two magnitudes (number of particles, size of particles)
- To hold Stokes number constant, particle density is decreased



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Case data

Case	Re	Pe	Stint	Stkol	al	alcl	alfit
St1	276.3	55.2	0.92	15.29	0.608	0.095	0.07271
St033	255.7	51.1	0.26	4.278	0.760	0.098	0.09560
St01	254.3	50.8	0.08	1.350	0.189	0.080	0.06572

Case	al/it	vp	Da	D	Rp	rhopm	rp*sqrtrho
St01	8.366	0.284	4.258	0.001	0.012	43.75	0.079
St033	7.954	0.332	1.672	0.001	0.012	13.75	0.044
St1	2.885	0.357	0.132	0.001	0.003	70.0	0.025

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