Simulation of high-intensity isotropic turbulence driven gas transfer

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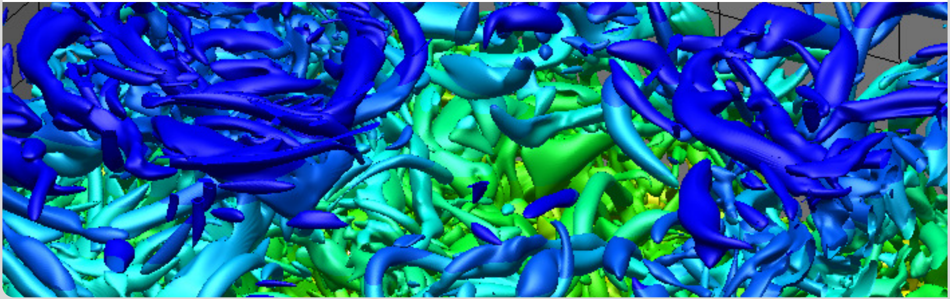
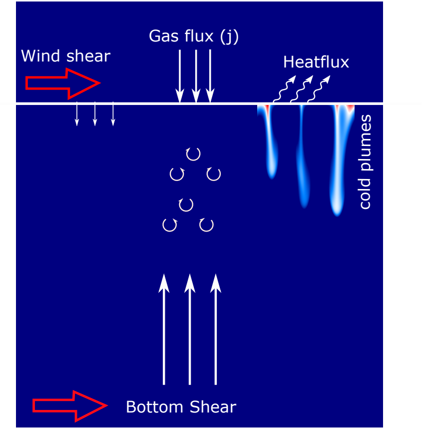


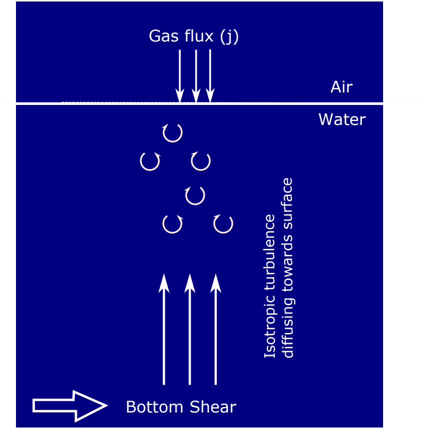
Isotropic turbulence driven gas transfer



Turbulence driving mechanisms

- Wind-shear
- Buoyancy
- Bottom-shear

Isotropic turbulence driven gas transfer



Turbulence driving mechanisms

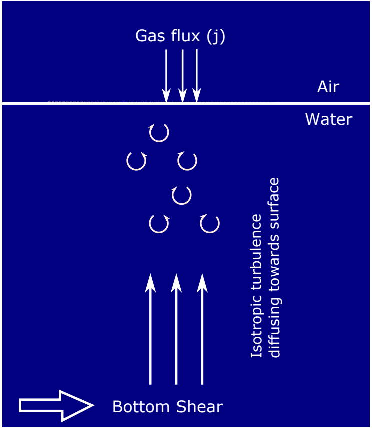
- Wind-shear
- Buoyancy
- Bottom-shear

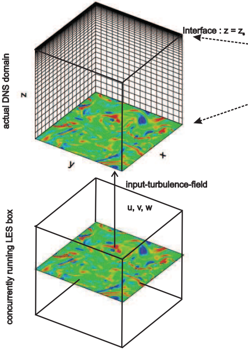
stream flow, low wind condition

http://repindonesiaraya.blogspot.de/2011/04/sungai-dan-letaknya.html

Isotropic turbulence

Convenient analogy to bottom-shear induced turbulent flow





numerical simulation

grid-stirred experiment

Parameterization

- Transfer velocity K_L

  $$j = K_L(C_{\text{interface}} - C_{\text{bulk}})$$

- Empirical and semi-empirical :

  K_L (wind speed)
  K_L (stream velocity)
  K_L (bed slope)
  $K_L(Re_b, Re_\tau, Re_T, Sc, \epsilon, etc.)$

- Detailed measurements :

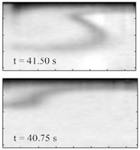
  $$j = -D\partial\langle c\rangle/\partial z + \langle c'w'\rangle$$

  $\rightarrow$ difficult

- Numerical simulations :

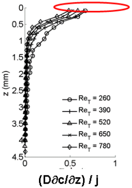
  Most DNS are limited to $Sc \leq 10$
  (while Sc of e.g. oxygen ≈ 500).

http://repindonesiaraya.blogspot.de/2011/04/sungai-dan-letaknya.html

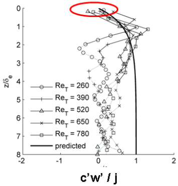


Oxygen concentration :
LIF image: 8mm x 4mm[1]

Molecular diffusion comp.

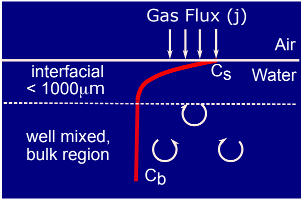


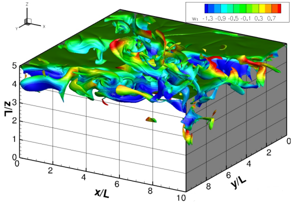
Turbulent mass flux comp.



[1] Herlina&Jirka 2008

Aim and scope





Simulation result: isosurface of 50% concentration saturation ($Sc = 20$)

- Generate highly-accurate data of the near surface flow and gas transfer dynamics using direct numerical simulations at realistic Schmidt numbers.

→ How are the dynamcis of the 3D vortical structures?

→ How is the instantaneous correlation between gas flux and near surface flow?

→ How does K_L scale with the turbulent Reynolds number R_T?

Numerical approach

Direct numerical simulations (DNS):

The set of equations (for fluid flow and scalar transport)

$$\frac{\partial u_i}{\partial x_j} = 0; \quad \frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{1}{Re}\frac{\partial^2 u_i}{\partial x_j \partial x_j}$$

$$\frac{\partial c}{\partial t} + \frac{\partial u_j c}{\partial x_j} = \frac{1}{ReSc}\left(\frac{\partial^2 c}{\partial x_j \partial x_j}\right)$$

is solved without any turbulence model.

This means all length and time scales need to be resolved.

→ We use the **in-house KCFlo**[(2)] **code**, which was specifically designed for resolving details of the gas transfer on a computational - feasible mesh size.

→ Dual meshing:
Gas concentration field is resolved on a finer mesh than the base-mesh used to resolve the velocity field.

[(2)] Kubrak et al. 2013

Computational set-up

- Boundary conditions:

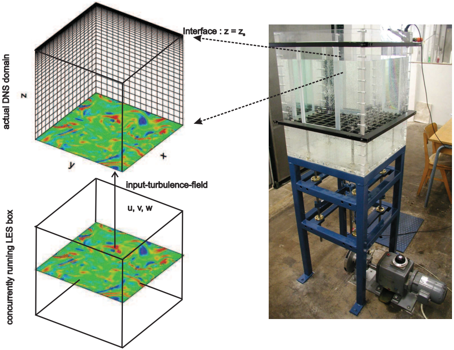
  Top: free-slip (clean)

  Side: periodic

  Bottom: flow-field copied from isobox

  $C_{\mathrm{interface}} = C_s$(saturated)

  Bottom: $\partial c / \partial z = 0$

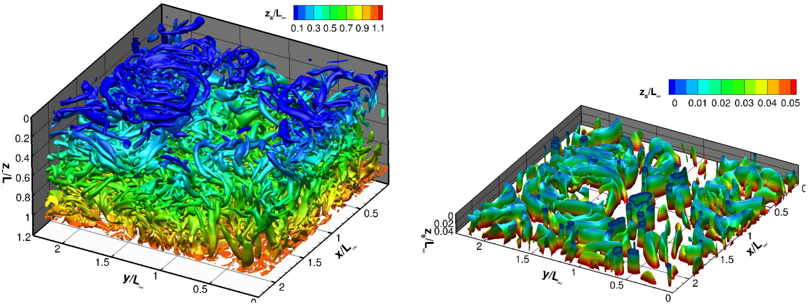


- Turbulent Reynolds number in the upper bulk $R_T = u_\infty 2L_\infty / \nu$
- Schmidt number $Sc = \nu / D$

R_T	Sc	Domain	Mesh Size	f_{RS}	L
$1440 - 1856$	$20; 500$	$20L \times 20L \times 5L$	$1024 \times 1024 \times 500$	$1; 5$	≈ 1 cm

Dynamics of vortical structures

Vortical structures



- At the bottom of domain, initially ‘randomly’ oriented vortical structures.
- Approaching the surface the flow becomes more and more 2D, and
- the vortical structures become either align or orthogonal to the surface.

Vortical structures and K_L

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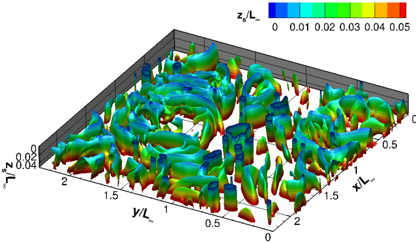
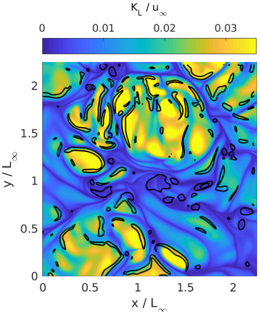
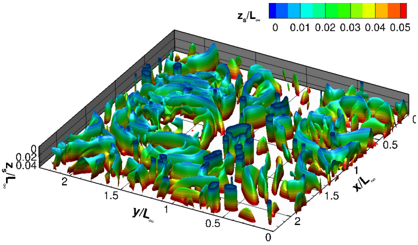




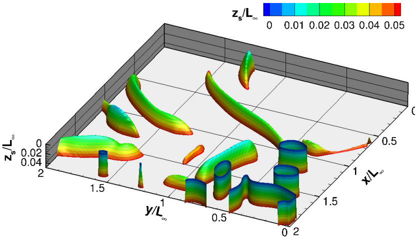
- Horizontally aligned slender vortical structures are found near the edges of high K_L-areas.
- Surface attached vortical structures are generally found in relatively low K_L-areas.

Vortical structures

$R_T = 1440$



$R_T = 507$



- Significantly more vortical structures in the higher R_T case.
- Significantly more fine-scale structures.

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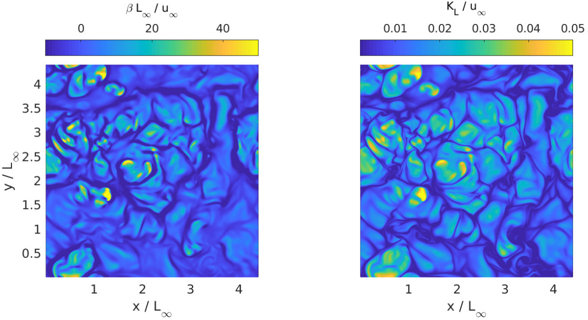
Correlation between gas flux and surface divergence

Surface divergence (β) and K_L at high R_T

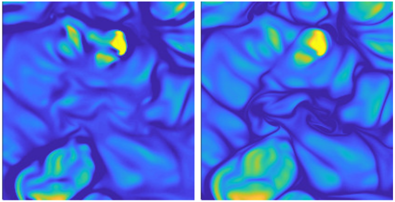


- Previous studies[(3)] confirmed that the surface divergence model, $K_L = c_\beta \sqrt{D\beta_{rms}}$, (although c_β varies).
- Here, footprints of size $\approx L_\infty$ show a good correlation between K_L and β.
- Footprints of fine-scale structures?

[(3)] e.g. McKenna & McGillis 2004; Magnaudet & Calmet 2006; Kermani et al. 2011;Turney 2016; Wissink & Herlina 2016

Surface divergence (β) and K_L at high R_T

β-contour K_L-contour



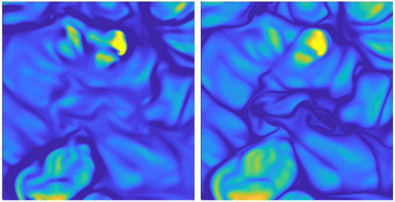
(zoomed-in view, $2L_\infty \times 2L_\infty$)

- Turbulence footprints of size $\approx L_\infty$ seen in K_L and β show a good correlation.
- Footprints of fine-scale structures are more clear in K_L contour than in β contour.

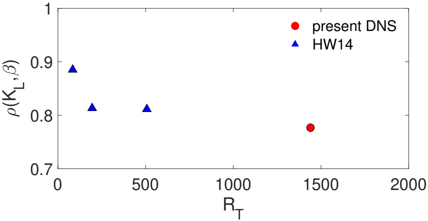
  $\rightarrow$ due to the difference in diffusivity.

Surface divergence (β) and K_L at high R_T

β-contour K_L-contour



(zoomed-in view, $2L_\infty \times 2L_\infty$)



- Turbulence footprints of size $\approx L_\infty$ seen in K_L and β show a good correlation.
- Footprints of fine-scale structures are more clear in K_L contour than in β contour.

  $\rightarrow$ due to the difference in diffusivity.

- High Reynolds number (R_T)

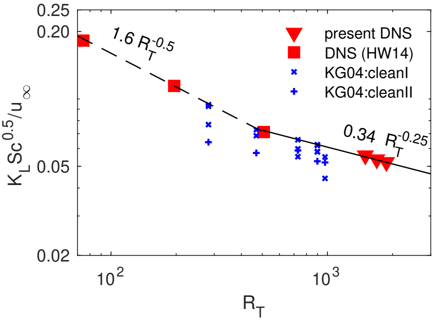
  $\rightarrow$ more fine-scale structures

  $\rightarrow$ $\rho(\beta, K_L)$ reduces

  $\rightarrow$ affects the applicability of the surface divergence model at high R_T (in agreement with Turney & Banerjee 2013).

Scaling of K_L with R_T

Scaling of transfer velocity



Two-regime model[4] :

Large eddy : $K_L \propto u_\infty Sc^{-1/2} R_T^{-1/2}$

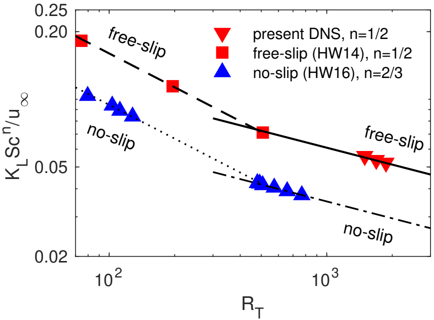
Small eddy : $K_L \propto u_\infty Sc^{-1/2} R_T^{-1/4}$

R_T is independent of the source of turbulence generation.

- Data confirms that at high R_T, mass transfer scales with the small-scales.
- Data confirms two-regime model.
- Data agree with the upper bound of KG04[5] experimental data

[4] Theofanous et al. 1976, 1984, [5] McKenna&McGillis 2004, [HW14] Herlina&Wissink 2014

Scaling of transfer velocity



Two-regime model[(6)] :

Large eddy : $K_L \propto u_\infty Sc^{-1/2} R_T^{-1/2}$

Small eddy : $K_L \propto u_\infty Sc^{-1/2} R_T^{-1/4}$

R_T is independent of the source of turbulence generation.

- No-slip cases (severely contaminated surface)
  - also two-regimes with transition at $R_T \approx 500$

$K_L \propto u_\infty Sc^{-2/3} \; R_T^{-1/2}$

$K_L \propto u_\infty Sc^{-2/3} \; R_T^{-1/4}$

[(6)] Theofanous et al. 1976, 1984, [(HW14)] Herlina&Wissink 2014, [(HW16)] Herlina&Wissink 2016

Summary

DNS of gas transfer at Sc up to 500 driven by high-intensity ($R_T = 1440 - 1856$) isotropic turbulence across a flat, clean interface:

- Surface parallel vortical structures contribute to vertical mixing, while surface-attached structures, merely mix already saturated fluid in the horizontal direction.
- Correlation between surface divergence β and K_L was found to become worse with increasing R_T.
- The importance of small-scale turbulent structures for $R_T \gtrsim 500$ was confirmed by the scaling

$$K_L Sc^n / u_\infty \propto R_T^{-0.25}.$$

- Combining the present results with our previous DNS, the existence of the small- and large-eddy regimes was confirmed numerically.

Acknowledgement

Deutsche Forschungsgemeinschaft (DFG)

Leibniz-Rechenzentrum (LRZ)

Helmholtz Water Network

Supplementary

Some numbers

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Isotropic turbulence driven mass transfer, $R_T = 1440 - 1856$

- Domain size : 20L x 20L x 5L (L$\approx$1cm)
- Base mesh : 1024 x 1024 x 500 (524×10^6 grid points)
- Refined mesh : 5120 x 5120 x 2500 (65.5×10^9 grid points)
- Number of processors : 20992
- Sc : 20, 500 (Refine=1, 5)
- On SuperMUC cluster at LRZ in Munich.
- Computation speed : 2.2 wall-clock /time-unit (only flow), 13 wall-clock /time-unit (scalar refine 5)
- Total disk space : 6.3TB
- Total CPUh : 18×10^6

Numerical scheme

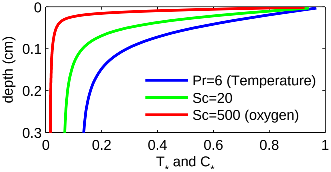
The Navier Stokes eqn is solved through direct numerical simulations using the in-house KCFlo code. The KCFlo code was specifically

designed for resolving details of the gas transfer on a ***computational - feasible*** mesh size, while avoiding spurious oscillations of the scalar quantity.

- Flow solver: 4th-order kinetic energy conserving discretisation for convection and 4th-order central discretisation for diffusion.
- Scalar solver: 5th-order WENO (Liu et al. 1994) for convection and 4th-order central discretisation for diffusion.

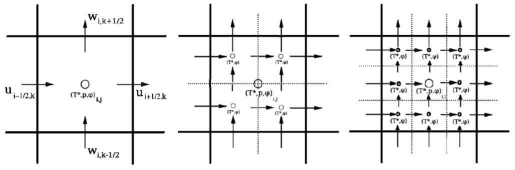
Dual-meshing strategy

Near the interface : grid size is determined by the smallest of the viscous, thermal and gas boundary layer thicknesses (δ).



$\delta_{gas} \approx 1/10\delta_T$

High Sc scalar field solved on a finer mesh than temperature and velocity field.



(a) Variables on a staggered mesh (b) Dual sub-mesh refined by factor R = 2 (c) Dual sub-mesh refined by factor R = 3

Kubrak, Herlina, Greve, Wissink JCP 2013

Limitation of experiments

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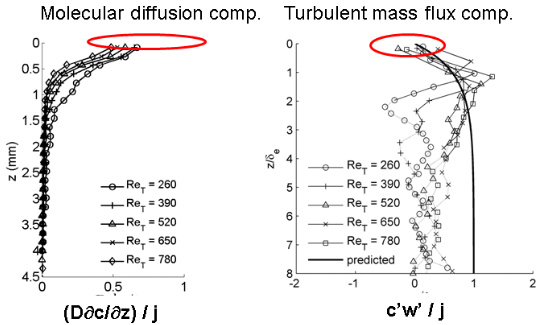


Diffusion comp.:

- dominant extremely near the surface.

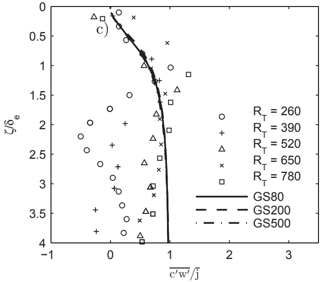
Turbulent comp.:

- Particular trend in the region z/d = 0 – 2
- c'w' ≈ j → contribution is significant

- difficulties in resolving the uppermost diffusive layer due to optical blurring and some degree of surface contamination
- quantification of c'w' becomes unreliable after z > 1.5 mm most likely due to insufficient laser intensity in the deeper bulk region
- only 2D information

Turbulent mass flux

HJ08 vs HW14



Run	Sc	Domain	Mesh Size	f_{RS}	R_T
GS80	$2-32$	$5L \times 5L \times 5L$	$128 \times 128 \times 300$	1	84
GS200	$2-32$	$5L \times 5L \times 3L$	$128 \times 128 \times 212$	1	195
GS500	$2-32$	$20L \times 20L \times 5L$	$512 \times 512 \times 300$	1	507
GS80R5	500	$5L \times 5L \times 5L$	$128 \times 128 \times 300$	5	84
GS200R5	500	$5L \times 5L \times 3L$	$128 \times 128 \times 212$	5	195

$L \approx 1$cm