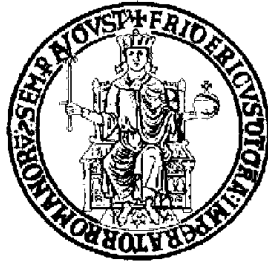


# Università degli Studi di Napoli Federico II



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## Dipartimento di Ingegneria Civile, Edile e Ambientale

*Classe delle Lauree Magistrali in Ingegneria per l'Ambiente e il  
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*Large Eddy Simulation on Chlorine Contact Tank:  
Hydrodynamics and Solute Transport*

Relatori:

Prof. Carlo Gualtieri

Prof. Thorsten Stoesser

Dr. Athanasios Angeloudis

Candidato:

Nicolò Viti

Matr. M67/239

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# CFD SIMULATION and VALIDATION ON CHLORINE CONTACT TANK: HYDRODYNAMICS AND SOLUTE TRANSPORT

Nicolò Viti

## Introduction

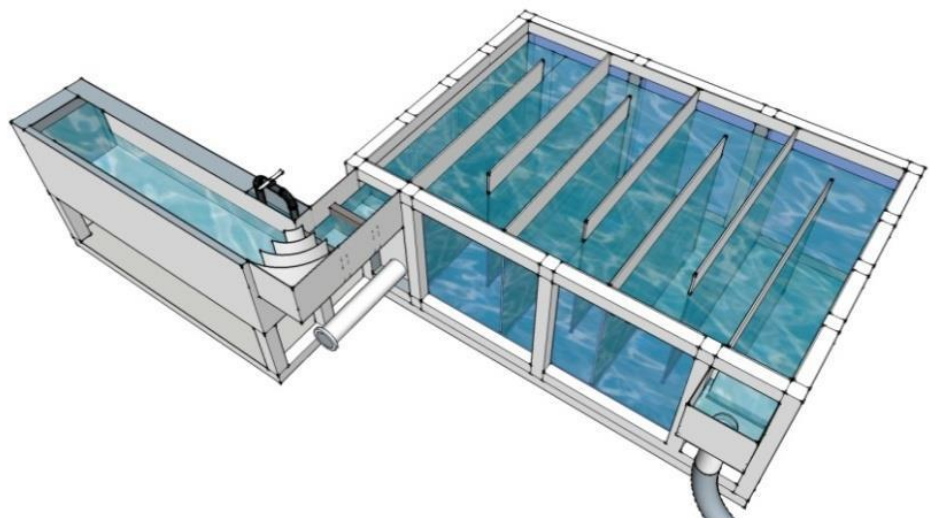
Hydrodynamics in contact tanks is known to strongly affect the process efficiency. A better understanding of the hydrodynamics and solute transport phenomena in water and wastewater treatment reactors has been undertaken by employing Reynolds-Averaged Navier-Stokes (RANS) equations and Large Eddy Simulation (LES) method comparing the simulation results to ADV experimental data. This study strives to address these questions:

- how can CFD be employed more efficiently to produce more accurate and useful results ?
- what really happens in the non-plug-flow chambers of a contact tank supposed to have a plug-flow behavior ?
- what are the effects of turbulence, recirculation zones and short-circuit zones on the solute transport ?

## Hydraulic aspects of Chlorine Contact Tanks

Serpentine contact tank units suggest plug flow to be the optimal hydrodynamic condition at which disinfection performance is maximized. However, previous studies indicate that flow exhibits a residence time distribution (RTD) which can be significantly distorted from what is dictated by plug flow. Over the years, there has been rising concern over the impact of such digressions from optimal hydraulic conditions on microbe inactivation and the regulation of potentially carcinogenic Disinfection By-Products (DBPs).

Fig. 1 - Three-Dimensional sketch of Contact Tank



## Large Eddy Simulation

With the growth of computing power and the advancement of computational models, the potential of contact tank water disinfection optimization by means of numerical modelling techniques can be assessed. In this study experimental data are compared with two three-dimensional Computational Fluid Dynamics (CFD) models (Reynolds-Averaged N-S and Large Eddy Simulation) set up to simulate the hydrodynamic and solute transport processes.

Large Eddy Simulation (LES) has been developed considering that large-scale is strongly energetic and boundary-condition dependent motion, on the other hand small-scale is more dissipative and universal and represents only a small part of the turbulent spectrum, thus it tends to be more isotropic and boundary-condition independent. According to this, LES calculates explicitly the motion of large-scales by solving the governing 3D time-dependent Navier-Stokes equations and treats the smaller-scale eddies, easier to model, with approximate models, called Sub Grid Scale Model (SGS Model).

## Experimental data availability

Velocity and turbulence measurements for the understanding of hydrodynamics have been acquired using Acoustic Doppler Velocimetry (ADV) in 1824 points. Tracer measurements take place at the top, middle and bottom of each compartment using Fluorometers which are calibrated to associate fluorescence intensity with the actual tracer concentration.

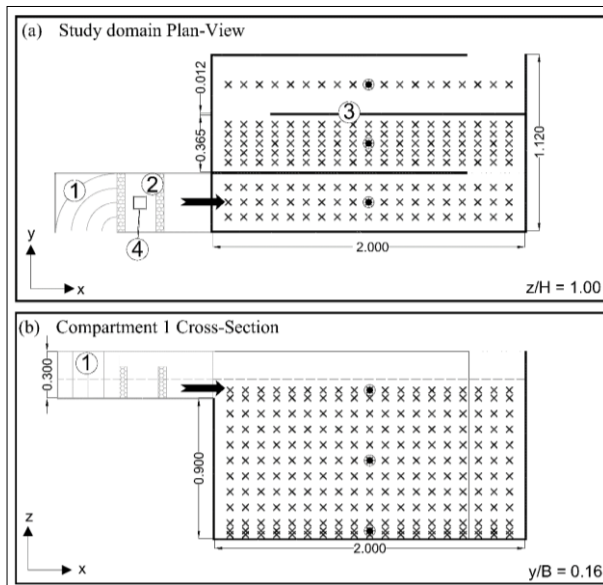
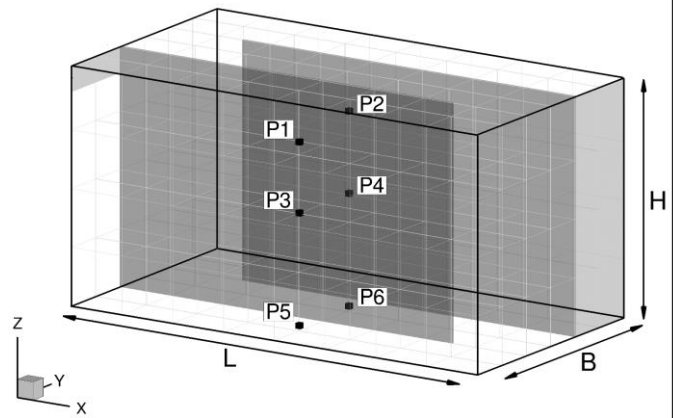
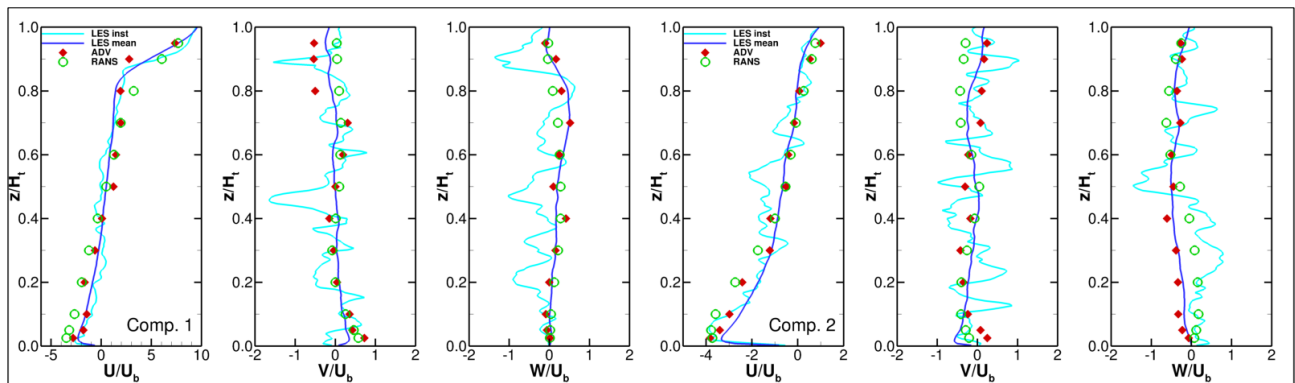


Fig. 2 – Experimental data sampling points:  
ADV left, Fluorometers right



## Hydrodynamics in Contact Tank: LES and RANS analysis

Hydrodynamics in contact tank is governed by unsteady large-scale flow structures due to flow separation that takes place in the junction between 1<sup>st</sup> and 2<sup>nd</sup> chamber and vortex formation among the first two compartments. The flow pattern corresponding to this regime suggests a scenario far from the plug-flow behaviour that a contact tank should have. Both RANS e LES simulations present a good accordance with experimental data in reproducing the flow field and the turbulent structures. Comparison between numerical data and experimental results has been undertaken calculating the percentage error of normalized velocity components in each section of both compartments: mean velocity profiles show a percentage error under 2% for both simulations, anyway thanks to LES the instantaneous values of velocity field is also provided. The covariance between velocity fluctuations in particular points of interest is also presented to better understand the turbulence phenomenon of the separated flow in the 1<sup>st</sup> junction.



LES and RANS percentage Error with ADV experimental data:

-0.85%	+1.85%	-0.10%	-0.52%	+1.21%	+1.19%	+0.37%	-0.12%	+0.92%	+0.66%	+0.16%	+0.26%
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Fig. 3 - LES (instantaneous and mean), RANS and ADV velocity profiles in the central line of 1° and 2° compartment with related percentage error against experimental data

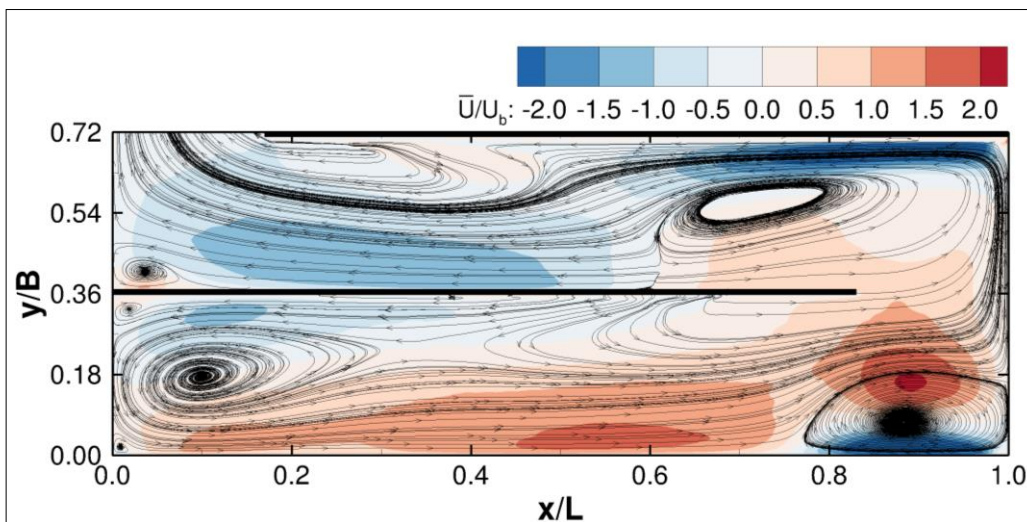


Fig. 4 –  
Horizontal slice  
at  $z/H = 0.60$

## Solute transport in Contact Tank: LES and RANS analysis

Solute transport in contact tank is strongly affected by hydrodynamics. It is evident the coexistence of tracer in both compartments due to the phenomenon of the separation of the flow: when the concentration is spreading in compartment 2, the massive recirculation zone in compartment 1 still holds the tracer for a greater time than the theoretical retention one. As a result, the presence of not-ideal plug flow condition is evident. The good performance of the simulations can be also investigated comparing the Residence Time Distribution (RTD) curves of numerical simulations with the experimental data. Both methodology are able to reproduce the shape and the trend of the curves, in particular LES is able to reproduce also the concentration fluctuations which are not captured by the RANS simulation.

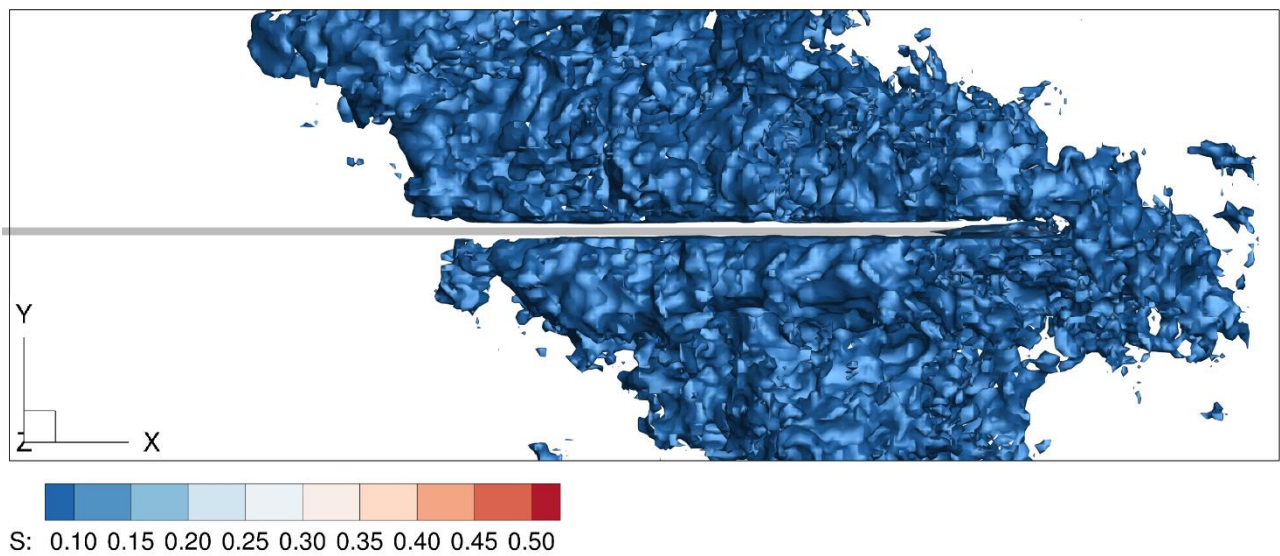


Fig. 5 - 2D iso-surface of instantaneous concentration at  $t=60s$

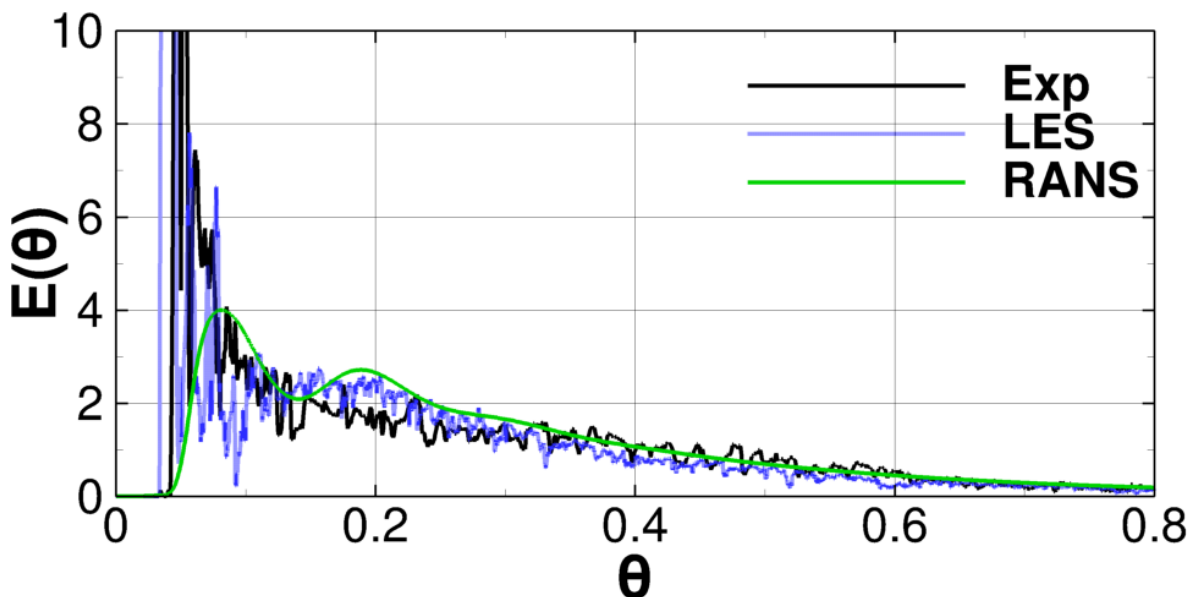


Fig. 6 – Residence Time Distribution (RTD) curves

## Concluding Remarks

The conclusions of this research from comparison between experimental data and numerical simulations show as the 3-D numerical models were able to reproduce the flow behavior very well and a good prediction of scalar transport throughout the tank was achieved. Testament of the ability of the modelling approaches is also reflected in the good match of simulated Residence Time Distribution curves with the experimental ones.

The main findings are outlined as follows:

- Turbulent mixing, dead-zones and short-circuiting in CTs affect solute transport and thus **disinfection efficiency** since the exposure of pathogens with the disinfectant is either too short (insufficient treatment) or too long, which can result in the production of excessive **disinfection by-products**
- Flow in CTs exhibits a Residence Time Distribution (**RTD**) which is often significantly different from that dictated by **plug flow** with resulting effects on the dispersion indicators
- The RANS widely used assumption of **isotropic turbulence** is **not** rightly **reliable** however unnecessary in LES
- **LES** offers a substantial increase in **accuracy** over time-averaged approaches (**RANS**) and delivers an enormous amount of information on the mean and instantaneous flow field