HYDRODYNAMIC MODELLING OF FLOW PATTERNS IN A VORTEX REACTOR - APPLICATION TO THE MIXING STUDY

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Abstract *– In the fuel reprocessing industry, an unbaffled magnetic rod-stirred multiphase reactor was developed for a precipitation operation. The flow generated in such a reactor is complex and the rotating agitator at the bottom of tank creates a vortex on the liquid surface. A Computational Fluid Dynamics (CFD) modelling is developed based on a Large Eddy Scale (LES) approach for turbulence effect simulation. The numerical simulations are performed in 3D using the Trio_U code developed at the Commissariat à l'Energie Atomique. The vortex study is based on an interface tracking method and the rotating magnetic rod is taken into account through a free IBC immersed boundary. The hydrodynamic modelling is in good agreement with Nagata's theory and will be validated from experimental data obtained by LDV measurements.*

INTRODUCTION

A multiphase reactor has been developed in the spent nuclear fuel reprocessing industry for use as a precipitator. It consists of an unbaffled cylindrical vessel stirred by a magnetic rod. The stirring action at the bottom of the vessel imparts a rotating movement to the fluid and forms a vortex at the surface. Precipitation reactions are very rapid, and are highly sensitive to mixing effects. In recent years CEA policy has been to model the entire operation, combining kinetic laws with the hydrodynamic behavior in the reactor.

Flows in stirred unbaffled vessels have not been widely discussed in the literature, unlike stirred baffled vessels, because they are less frequently used in processes. Their mixing performance is significantly lower due to the predominance of the tangential velocity over the axial and radial velocity components. Without counter-impellers, however, fluid rotation leads to the formation of a vortex that distorts the free surface; some applications can take advantage of this vortex. In the precipitator considered here, this configuration limits scaling by maintaining potentially adhering particles away from the walls, and thus facilitates maintenance procedures that are particularly demanding in the nuclear industry [1]. This device is known as a “vortex reactor”.

Moreover, all the studies described in the literature concern conventional impellers, either radial (turbines, flat- or pitched-blade stirrers) or axial (helical impellers), none of which corresponds to a magnetic rod rotating at the bottom of the vessel.

OVERVIEW OF COMPUTATIONS

According to the Rankine's combined vortex description, the hydrodynamics in an unbaffled stirred tank reactor is characterized by the presence of two macromixing zones. The liquid near the axis rotates as a solid cylinder with an angular velocity closed to the agitator one, whereas the outside liquid behaves as a free vortex [2]. Due to the predominance of the circulation flow around the impeller axis, the turbulence is highly anisotropic. Then, the classical statistical turbulence models (Reynolds-Average Navier-Stokes RANS-like models) cannot be applied. The turbulence transport simulation can be achieved using the Large Eddy Simulation (LES) approach which resolves the largest scales using filter and gives the unsteady flow field taking into account the real movement of the stirrer.

The current investigations seek to develop unsteady-state models based on the Large Eddy Simulation using the Trio_U code developed by CEA-Grenoble [3].

A simplified geometry, shown on Fig. 1, is used for this study. It consists of a cylindrical glass unbaffled tank with a T diameter, a H height and a D length magnetic rod. The ratio between the diameters of the tank and the rod D/T is equal to 0.47. The tank is supposed to be filled with water.

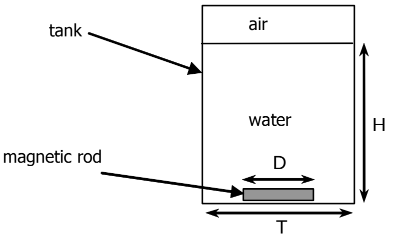

Fig. 1. Geometry used for the CFD modelling

An unstructured grid is realised with about 200 000 tetrahedral elements (see Figure 2).

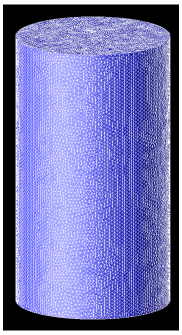

Fig. 2. Unstructured grid with tetrahedral elements

The air/water interface is simulated by a discrete front-tracking method and defined by a moving Lagrangian mesh independent of the Eulerian mesh of the calculation domain. It moves according to the flow hydrodynamics. The magnetic rod rotation kinetics are taken into account by an immersed interface method [4]. The displacement rate of the points on the interface is controlled, and reproduces the rotational movement of the stirrer. The submesh turbulence model used is a functional-modelling-like unsteady model, the WALE model [5].
The initial conditions of this calculation consider a fluid at rest with a horizontal free surface. At the initial instant the magnetic rod is driven to the required constant rotation speed with a Reynolds number of about 7 10^4.

RESULTS AND DISCUSSION

Inducing fluid flow

The entire fluid volume cannot be placed in movement instantaneously: 15 seconds are necessary for the volume fluid to reach steady-state kinetic energy conditions (see Fig. 3).

The air/water interface simulation method allows us to observe the continuous movement of the free surface after formation of the vortex, unlike a statistical approach in which the free surface is considered fixed. The vortex follows the main rotational movement of the flow, and the interface is therefore not exactly axisymmetric in the vortex zone: its tip exhibits slight precessional motion.

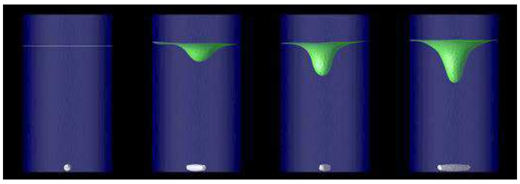

Fig. 3. Vortex formation: Initial state and first few seconds of transient phase

The calculated free surface is consistent with Nagata's relation [6], as shown in Fig. 4 which compares the vortex profiles calculated at different moments with the theoretical profile.

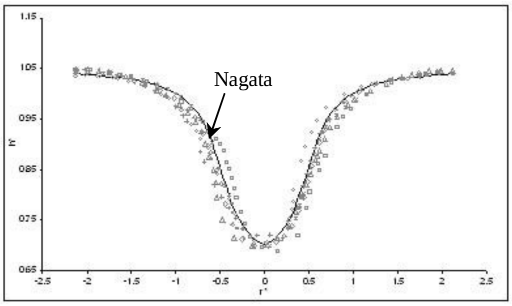

Fig. 4. Comparison of calculated vortex profiles with Nagata's model

Instantaneous velocities provided by large-scale simulation

The main flow comprises fluid rotation around the vessel symmetry axis, in which the tangential velocity component predominates. However, the tangential velocity norm varies in space and time with the rod position. The fluid is periodically discharged radially by the rod, forming structures superimposed on one other over the full height of the reactor. These moving structures vary approximately synchronously with the movement of the stirrer. The velocity vector field shown in Fig. 5 on a reactor midplane at different times demonstrates the displacement of these structures.

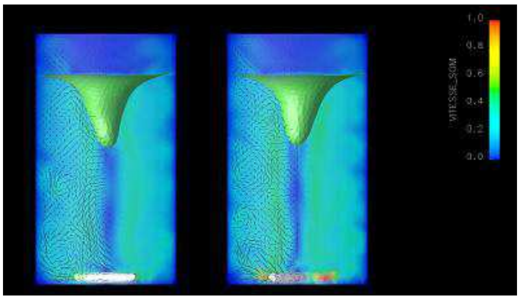

Fig. 5. Vector fields at two different instants on a reactor midplane

Representing the eddy structures based on a turbulence criterion shows a dominant vertical central structure surrounded by smaller secondary structures that exhibit not only helical rotational movement around the vessel centerline, but also upward motion from the bottom toward the vortex (see Fig. 6). The secondary structures are in the free vortex zone.

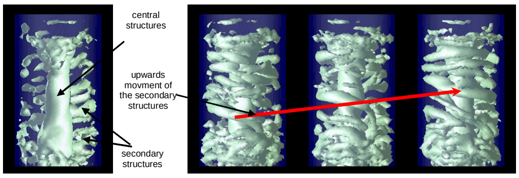

Fig. 6. Representation of turbulent flow structures

Experimental acquisition of velocity fields by Laser Doppler Velocimetry (LDV) and observations of the free flow surface are currently in progress to validate the simulations.

Tracer path

Simulating the injection of a tracer visualizes the preferential path followed by a fluid particle depending on the initial feed location (see Fig. 7). The computational simulations reproduce the experimental observations (see Fig. 8).

A passive tracer injected into the forced vortex remains confined inside until it reaches the stirrer; then it diffuses into the free vortex. On the contrary, when the passive tracer is supplied in the free vortex, the tracer is diluted into the whole volume of the reactor.

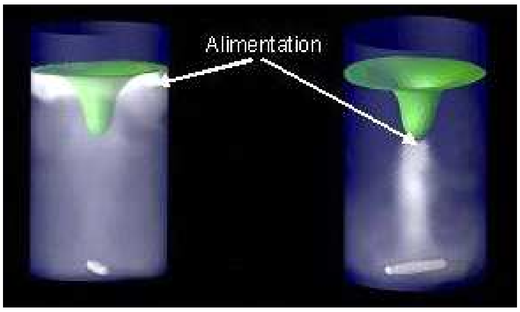

Fig. 7. Tracer path depending on point of injection - CFD simulation

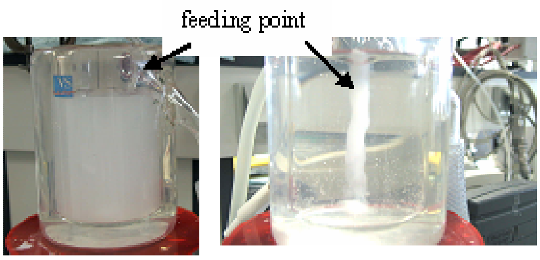

Fig. 8. Tracer path depending on point of injection - Experiments

CONCLUSIONS

The LES approach using Trio_U code is successfully applied to simulate with a high accuracy degree the unbaffled stirred tank precipitator. The hydrodynamic modelling is in good agreement with Nagata's theory and will be validated from experimental data obtained by LDV measurements. The LES simulations allow us to get unsteady velocity and turbulence fields according to the magnetic rod position.

This hydrodynamic study appears to be an important step for the precipitation operation simulation. Indeed, the CFD modelling developed will be combined with the population balance in order to have a better understanding of the phenomena developed into the reactor during the precipitation process. Furthermore, a sub-grid model is developed with the LES approach in order to take into account a chemical reaction sensitive to micromixing phenomena. The computer simulation is an important tool for the design, the optimisation and scale-up of new geometries, especially in nuclear environment where experiments are limited.

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