

Avoiding Explosive Outcomes



A mixing vessel in the test facility at ADI

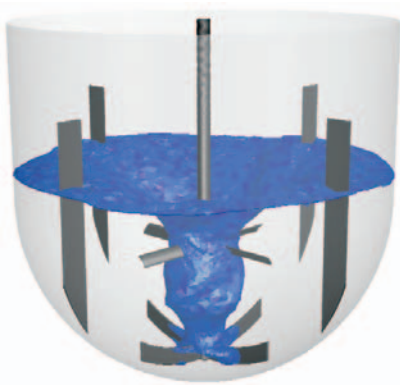
By Jimmy Lea, ADI, Garden Island, Australia, and
Adesoji A. Adesina, Department of Chemical Engineering, The University of New South Wales, Sydney, Australia

AUSTRALIAN DEFENCE INDUSTRIES (ADI), through its Land Ordnance Unit, manufactures energetic products, mostly for military applications. There are inherent risks in the manufacture of high explosives such as RDX and TNT and their derivatives. Consequently, it is not always convenient to optimize the unit operation by building a pilot-scale version or to conduct physical experiments in the actual plants. Inappropriate experiments or small errors made in such sensitive conditions may lead to catastrophic losses. Apart from the safety aspects, stopping production to conduct experiments may be economically prohibitive. CFD has therefore been introduced to help identify the underlying cause of inconsistent production quality.

Cyclotol, a military high explosive, is produced by mixing cyclo-1,3,5-trimethylene-2,4,6-trinitramine (or RDX – Research Department explosive) and 2,4,6-trinitrotoluene (TNT) to specified ratios. RDX slurry (water and RDX solid particles) is fed into molten TNT in a mixing tank equipped with a double-impeller and maintained at constant temperature. There are four non-penetrating phases in this system: the RDX particles, the heaviest component; molten TNT; water; and air (above the free surface).

At the start of the process, the TNT is melted in the vessel with the impeller speed at 40 rpm. The impeller speed is increased to 58 rpm when the RDX slurry is introduced. The speed is reduced to 40 rpm and mixing takes place for 10 minutes within a temperature range of 85 to 100 °C. The speed is then reduced further to 10 rpm for 5 to 10 minutes so that the product can reach the proper density. At the end of this period, the highly explosive mixture is transferred to the next unit operation to be further processed. Ideally, the transferred liquid should be water-free cyclotol.

There are several complicating factors that contribute to the final product quality, and these are governed by the impeller speed. If it is set too high at any time during the process, the drawdown vortex formed will cause the entrainment of water. If it is set too low, on the other hand, the suspension uniformity will suffer because the RDX particles are heavier than molten TNT. The impeller speed during the tank transfer is also important, since it can impact the amount of water that gets entrained at the outlet. The objective of the CFD work is to prescribe a set of operating conditions that help avoid or mitigate these issues while satisfying process safety and profitability. The



An iso-surface of water volume fraction illustrates the drawdown at 20 rpm

MRF model was used in FLUENT to simulate the motion of the impeller in the baffled vessel, and the mixture multiphase model was used to account for the constituents. The realizable $k-\epsilon$ model was used for turbulence.

The first objective was to study water drawdown as a function of impeller speed. Simulations of a 3-phase system in the vessel consisting of cyclotol mixture at the bottom, water floating above it, and air on top were conducted. Results showed that water was drawn down to the top impeller at impeller speeds as low as 10 rpm. At higher speeds, the water was drawn down further into the cyclotol mixture. The ease of water drawdown can be attributed to the close cyclotol-to-water density ratio (about 1.7). These CFD results provide the underlying reason for the fluctuations in the density readings observed during product mixing.

The second objective was to assess the ability of the mixer to suspend RDX particles in molten TNT at 85°C, as the impeller speed was varied from 0 to 40 rpm. With the impellers at rest, the particles collected

in the base of the vessel. As the speed increased, more and more particles became suspended, and the cloud height increased, as expected. While a homogeneous suspension of RDX in molten TNT was not attained at 20 rpm, a significant improvement was seen at 30 rpm, where localized clusters of particles diffused and the cloud height reached about 80% of the liquid level in the tank. Further improvement was achieved at 40 rpm. This set of results explains why production personnel experienced product variations from batch to batch when the impellers were rotating at only 10 rpm during the critical mixing phase of the process.

The third objective was to characterize the water entrainment during the emptying process, in hopes of identifying the lowest allowable level that the cyclotol mixture can reach before the emptying valve is closed. In practice, the cyclotol/water interface must not fall below 20% of the initial liquid height. Under these conditions, some water (16% by volume) does reach the tank bottom, immediately above the bottom outlet. During the transfer of the explosive mixture, this water

will be carried over to the next unit operation, and could potentially compromise the final product quality.

In summarizing these results, good particle suspension can be achieved at a minimum impeller speed of 40 rpm, but this exceeds the constraint stipulating a maximum speed of 20 rpm to avoid water drawdown. A change in the design of the mixing tank is therefore required to prevent water drawdown and achieve a homogeneous RDX suspension. During the next phase of the project, several design changes will be studied, including the use of different impellers and their locations in the tank. Although CFD simulation is not a substitute for physical experiments, it can significantly reduce the number of actual experiments that need to be conducted. This enables the redesigning of this mixing tank to be expedited while minimizing the associated costs. ■

“CFD technology has provided the engineers with information not previously possible. This has enhanced our understanding of the process and hence shed some light on an ongoing problem of excessive variation in final product composition.”

– Paul Flavel
Manufacturing Operations Manager
ADI-Mulwala

Acknowledgments

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Suggested Reading

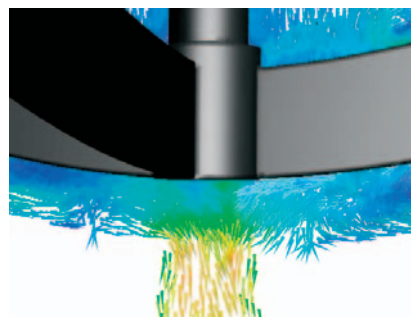
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2. Lea, J.; Gehrig, A.; Flavel, P.; and Adesina, A.: The CFD modelling and simulation of a nitration unit employed for the manufacture of military propellants. ICCHMT, Paris, France, May 17-20, 2005.



Volume fraction of RDX particles at 20 rpm



Volume fraction of water with the cyclotol/water interface at 20% of the liquid height



Water entrainment below the semi-anchor impeller at the base of the vessel