## Mechanochemical Destruction of DDTs with Fe-Zn Bimetal in a High-Energy Planetary Ball Mill

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**Background/Objectives.** Mechanochemical destruction (MCD) has been proposed as a promising, non-combustion technology for the safe disposal of toxic, halogenated, organic pollutants. In the study presented, additives including Fe, Zn, Fe-Zn bimetal and CaO were tested for their effectiveness to treat DDTs by MCD. Discrete element method (DEM) modelling, a mathematical tool, provides a useful approach to simulate the ball motion in the milling vial and allow the study of the relationship between impact energy of mill balls and rate constant of MCD.

Approach/Activities. To examine the effectiveness of different reagents, CaO, iron powder, zinc powder and mixed iron-zinc powder were chosen as reagents for MC destruction of DDTs. A simplified model for the grinding motion was created in EDEM software (DEM Solutions, UK). The milling balls were replaced by spherical discrete elements. The milling vial was represented as a compound object, consisting of top and bottom disks and a cylinder as the vial wall. The dimensions of milling balls and vials were equal to actual experimental setup size. A mathematical kinetic model on the relation between removal rate constant and the two main factors was determined for prediction and optimization of operation conditions. In addition, water-soluble chloride, XRD, FITR and Raman spectra measurements were carried out to study the potential mechanism of DDT destruction by Fe-Zn bimetal-based MCD process.

Results/Lessons Learned. The results showed that Fe-Zn bimetal was the most efficient additive, with 98% of DDTs removed after 4 hours. For the presented grinding device, the optimal rotation speed range was 200 to 400 rpm. A more precise, linear correlation was observed between rate constant and normal impact energy rather than with total impact energy. Vertical collision between mill balls and the vial wall is proposed to play a more important role in MCD reaction. The specific energy dose instead of milling intensity are key factors that influence the removal efficiency of DDTs in MCD reaction. The process of mechanochemical ball milling is the breaking down of the DDT's structure, the cleavage of C-Cl bonds, the destruction of the benzene ring and the generation of inorganic carbon, revealing that dechlorination and carbonization occurred during the treatment reaction. Zinc is preferentially consumed during milling.