Modeling and uncertainty analysis of dust explosion

Zoltan K. NAGY,

Davidson School of Chemical Engineering
Purdue University, West Lafayette, IN
December 12, 2018

Purdue Process Safety and Assurance Center (P2SAC)

Importance of dust explosions

“Devastating dust explosions have occurred in pharmaceutical facilities around the world, destroying equipment, injuring or taking lives and halting businesses. It's not a risk worth taking. During the handling, storage and processing of pharmaceutical raw materials, the explosion risk of bulk powders is always present”

European Pharmaceutical Manufacturer Magazine, 14 March 2014, Protecting Pharma from Dust Explosions.

Image: West Pharmaceutical Services Dust Explosion and Fire (01/28/2003) - six deaths, dozens of injuries, and hundreds of job losses
Project Objectives

- Develop a mechanistic multi-scale model of dust explosion
- Using a reaction engineering approach and a PBM-CFD framework
- Implement a numerical efficient solution approach using parallelized GPU-based implementation
- Apply a fast uncertainty propagation approach
- Parameter identification with corresponding parametric and structural uncertainties (due to reaction kinetics)
- Uncertainty analysis and robust optimization for reactive and preventive safety measures
- Equipment and material specific risk analysis framework based on explosive index (EI) and suggest more robust design and recommended controls

Proposed Multi-scale approach for dust explosion modeling

- Effect of dust size and CSD
- Effect of dust shape (spherical vs. needle)
- Effect of dust agglomeration
- Effect of turbulence
- Effect of composition (API/excipient)

- Combined PBM-CFD approach
- Use CFD concepts for turbulent, multiphase, chemically reacting flows
- Based on material properties of fuel and oxidizer at particle scale and at cloud scale CFD is applied
- More generalized and less assumptions, leading to better fundamental understanding of dust explosion
- Efficient implementation using parallelized solution on GPUs to be able to simulate the fast process (~1s)
- Use model for mechanistic understanding and design of robust mitigation strategies (e.g. venting and automatic dust explosion suppression – fast acting fire distinguishers)
Efficient uncertainty propagation

- Uncertainty in model parameters: $\theta = \hat{\theta} + \delta \theta$
- Described by a hyper-ellipsoid: $\mathcal{E}_\theta = \{\theta : (\theta - \hat{\theta})^T V_\theta^{-1} (\theta - \hat{\theta}) \leq \chi^2_n(\alpha)\}$
- Uncertainty in output: $\psi = \hat{\psi} + \delta \psi$ characterized by $\mathcal{E}_\psi$ and $V_\psi$
- Analytical computation of variance, using PSE or PCE:

\[
\begin{align*}
\delta \psi &= L \delta \theta + \frac{1}{2} \delta \theta^T M \delta \theta + \ldots \\
L(t) &= \left(\frac{\partial \psi(t)}{\partial \theta}\right)_{\hat{\theta},\hat{\psi}(t)} \\
M(t) &= \left(\frac{\partial^2 \psi}{\partial \theta^2}\right)_{\hat{\theta},\hat{\psi}(t)} \\
\psi^{(i)} &= a_1^{(i)} \Gamma_1(\theta_i) + \left(\text{constant terms}\right) + \sum_{i=1}^{n_1} a_2^{(i)} \Gamma_2(\theta_i, \theta_i) + \ldots \\
&\quad + \sum_{i=1}^{n_2} \sum_{j=1}^{n_1} a_3^{ij} \Gamma_3(\theta_i, \theta_j, \theta_j) + \ldots
\end{align*}
\]

Efficient uncertainty propagation (power series and polynomial chaos)

Uncertainty propagation & identification of attainable regions and safest operating regimes

- Monte Carlo simulation with nonlinear model (simulation time 64 h)
- Distributional robustness analysis using PCE (simulation time 0.2 s)

Low sensitivity – safest operating condition