Modeling and uncertainty analysis of dust explosion

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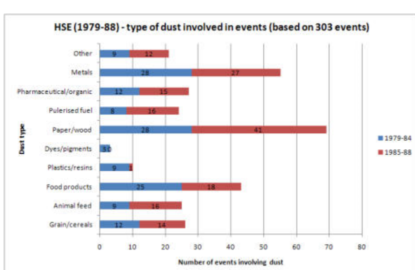
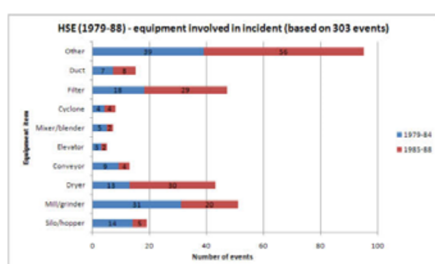
Importance of dust explosions

"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 (01/29/2003) - 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

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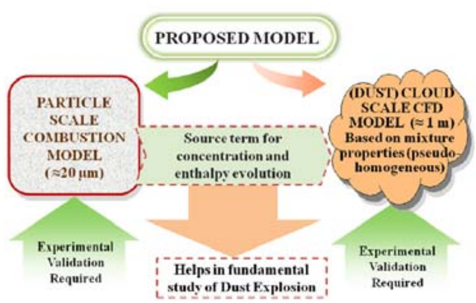
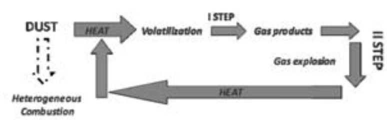
Proposed Multi-scale approach for dust explosion modeling





- 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)

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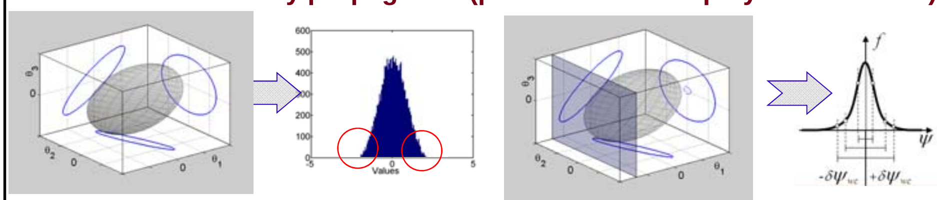
Efficient uncertainty propagation

- **Uncertainty in model parameters:** $\theta = \hat{\theta} + \delta\theta$
- **Described by a hyper-ellipsoid:** $\varepsilon_\theta = \{\theta : (\theta - \hat{\theta})^T \mathbf{V}_\theta^{-1} (\theta - \hat{\theta}) \le \chi_n^2(\alpha)\}$
- **Uncertainty in output:** $\psi = \hat{\psi} + \delta\psi$ **characterized by** $\mathcal{E}[\psi]$ **and** V_ψ
- **Analytical computation of variance, using PSE or PCE:**

$$\delta\psi = L\delta\theta + \frac{1}{2}\delta\theta^T \mathbf{M}\delta\theta + \ldots \qquad L(t) = \left(\frac{\partial\psi(t)}{\partial\theta}\right)_{\hat{\theta},u(t)} \in \mathbb{R}^{n_\theta} \quad \mathbf{M}(t) = \left(\frac{\partial^2\psi}{\partial\theta^2}\right)_{\hat{\theta},u(t)} \in \mathbb{R}^{n_\theta \times n_\theta}$$

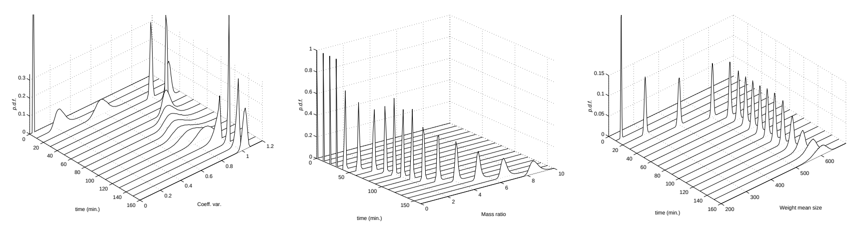
$$\psi^{(d)} = \underbrace{a_o^{(d)}\Gamma_o}_{constant} + \underbrace{\sum_{i_1=1}^{n_\theta} a_{i_1}^{(d)}\Gamma_1(\theta_{i_1})}_{first\,order\,terms} + \underbrace{\sum_{i_1=1}^{n_\theta}\sum_{i_2=1}^{i_1} a_{i_1 i_2}^{(d)}\Gamma_2(\theta_{i_1},\theta_{i_2})}_{second\,order\,terms} + \underbrace{\sum_{i_1=1}^{n_\theta}\sum_{i_2=1}^{i_1}\sum_{i_3=1}^{i_2} a_{i_1 i_2 i_3}^{(d)}\Gamma_3(\theta_{i_1},\theta_{i_2},\theta_{i_3})}_{third\,order\,terms} + \ldots$$

- **Efficient uncertainty propagation (power series and polynomial chaos)**

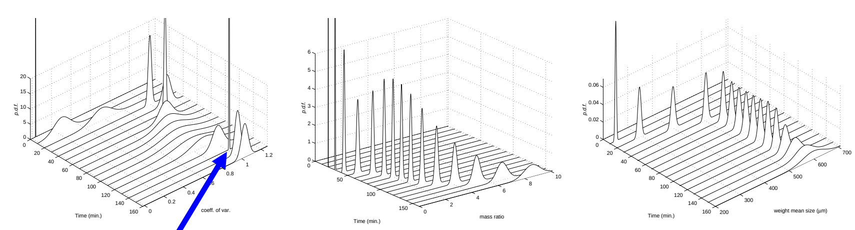


Uncertainty propagation & identification of attainable regions and safest operating regimes

- 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