Study of Thermal and Volatilization Induced Primary Fragmentation and Statistics of Coal Particles Subjected to Plasma Initiated Detonation using Weibull Theory

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Introduction

Detonation combustion of coal holds promise of higher system and combustion efficiencies.

Primary fragmentation of coal in the combustion process is known to substantially impact efficiency.

Coal is likely to remain an important energy source and hence improvements in coal combustion technology will have major impact.

Coal combustion is composed of four major stages

- Thermal heating
- Devolatilization
- Defragmentation due to thermal and/ volatilization
- Burning

The work presented here reports analytical and numerical studies on thermal and volatilization induced fragmentation of coal when subjected to a detonation wave.
Present Work

• A detonation wave is generated using a plasma cartridge at one end of a detonation tube.
• Response of coal particle to detonation waves of Mach numbers 3 to 8 are studied.
• Thermal and volatilization induced primary fragmentation under detonation condition is aim of this work.
• Stresses induced due to combined thermal and volatilization effects are calculated.
• Convective and radiative boundary condition is used.
• Numerical code was written and the solution obtained is compared with analytical solution.
• Particle is assumed fractured when maximum principal stress exceeds ultimate strength.
I started with developing HTM of simple constant temperature boundary condition using analytical methods. I predicted particle fracture time and location due to thermal stress only using failure criteria suggested by various failure theories.

Applied this model to solve more realistic boundary conditions; convective and radiative boundary conditions.

After successfully developing HTM analytically I moved on to develop numerical model for solution of more complex problem.

I developed CFD code to solve convective and radiative boundary condition and compared it with analytical solutions. It matched with minimum error.

After developing HTM numerically I developed VM of volatile matter.
• I linked HTM and VM with SMM and obtained principal stresses developed in coal particle. Here it ends the linking of all models and gives DSM.

• After successfully developing DSM I developed FCM using Weibull’s WLT. This model is capable of giving fragmentation time, fragmentation location, temperature at the time of fragmentation, volatilization matter present at fracture, flow of volatile at fracture, pressure at fracture.

• This ends complete PFM which includes HTM, VM, SMM, DSM and FCM.

• After developing PFM for single coal particle I developed SM which is capable of giving me average, Standard Deviation, PDF, CDF of the mixture of different size coal particles.
Unsteady heat conduction equation with spherical symmetry is.

\[
\frac{1}{r^2} \frac{\partial}{\partial r} \left( kr^2 \frac{\partial T(r, t)}{\partial r} \right) = \rho C_p \frac{\partial T(r, t)}{\partial t}
\]  

(1)

And the boundary conditions are:

\[
T(r_o, t) = T_\infty
\]

(2)

where \( T_\infty \) is the skin temperature induced by the detonation wave. And

\[
\frac{\partial T}{\partial r} \bigg|_{r=0} = 0
\]

(3)

The initial condition is:

\[
T(r, 0) = T_i
\]

(4)
Solution can be obtained by two different analytical techniques

Solution from Separation of Variable technique

\[
\tau(R, \theta) = \frac{T(r, t) - T_\infty}{T_i - T_\infty} = \sum_{m=1}^{\infty} \frac{-2(-1)^m}{\lambda_m R} \sin(\lambda_m R)e^{-\lambda_m^2 \theta} \tag{5}
\]

where \(\sin \lambda_m = 0\) is the eigen condition and \(\lambda_m = m\pi\) \((m = 1, 2, \ldots)\) are the eigenvalues.

And solution from Laplace Transform technique

\[
\tau(R, \theta) = \frac{T(r, t) - T_\infty}{T_i - T_\infty} = \sum_{m=1}^{\infty} \frac{-2(-1)^m}{\lambda_m R} \sin(\lambda_m R)e^{-\lambda_m^2 \theta} \tag{6}
\]

Where eigen condition is \(\sinh(\sqrt{z}) = 0\). The eigen values are the poles of the function \(f(z)\), which are, \(z = -\lambda_m^2 = -m^2\pi^2\)
Temperature profile

Figure: Coal particle temperature distribution
Maximum Principal Stress Theory

This theory was suggested by Rankine. The theory is based on calculating maximum principal stresses induced in the coal particle and comparing it with ultimate strength.

\[
\sigma_{n1,2} = \frac{\sigma_r}{2} \pm \sqrt{\left(\frac{\sigma_r}{2}\right)^2 + \sigma_t^2} \geq \frac{\sigma_{uu}}{N}
\]

Figure: Developed thermal stress distribution at detonation Mach no. 3
Maximum Principal Stress Theory

Figure: Developed thermal stress distribution at detonation Mach no. 5

(a) 50 µ
(b) 100 µ
(c) 150 µ
Maximum Principal Stress Theory

Figure: Developed thermal stress distribution at detonation Mach no. 7

(a) 50 μ
(b) 100 μ
(c) 150 μ
Maximum Principal Strain Theory

This theory was developed by Saint Venant. According to this theory, the failure or yielding occurs at a point in the member when the maximum principal strain in the bi-axial stress system reaches the limiting value of strain.

\[ \sigma_{n1} - \nu \sigma_{n2} = \frac{\sigma_{uu}}{N} \]

Figure: Developed thermal stress distribution at the detonation Mach no. 3

(a) 50 \( \mu \)  
(b) 100 \( \mu \)  
(c) 150 \( \mu \)
Figure: Developed thermal stress distribution at the detonation Mach no. 5

(a) 50 µ
(b) 100 µ
(c) 150 µ
Figure: Developed thermal stress distribution at the detonation Mach no. 7

(a) 50 µ  (b) 100 µ  (c) 150 µ
Maximum strain is given by

$$\epsilon_{max} = \frac{\sigma_{n1}}{E} - \frac{\nu \sigma_{n2}}{E}$$

(a) 50 µ  
(b) 100 µ  
(c) 150 µ

**Figure:** Maximum strain distribution at the detonation Mach no. 3
Figure: Maximum strain distribution at the detonation Mach no. 5

(a) 50 $\mu$
(b) 100 $\mu$
(c) 150 $\mu$
**Principal Strain**

**Figure**: Maximum strain distribution at the detonation Mach no. 7

(a) 50 µ  
(b) 100 µ  
(c) 150 µ
Maximum Shear Stress Theory

This theory was suggested by Guest and Tresca. The theory is based on calculating maximum shear stresses induced in the coal particle and comparing it with ultimate strength.

\[ \tau_{max} = \sqrt{\left( \frac{\sigma_r}{2} \right)^2 + \sigma_t^2} = \frac{\sigma_{uu}}{2 \times N} \]

(a) 50 \( \mu \)  
(b) 100 \( \mu \)  
(c) 150 \( \mu \)

**Figure:** Developed thermal shear stress distribution at detonation Mach no. 3
Maximum Shear Stress Theory

Figure: Developed thermal shear stress distribution at detonation Mach no. 5

(a) 50 $\mu$
(b) 100 $\mu$
(c) 150 $\mu$
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Maximum Shear Stress Theory

Figure: Developed thermal shear stress distribution at detonation Mach no. 7

(a) 50 $\mu$
(b) 100 $\mu$
(c) 150 $\mu$
Maximum Distortion Energy Theory

This theory was suggested by Hencky and Von Mises. According to this theory, the failure or yielding occurs at a point in a member when the distortion strain energy per unit volume, also called as shear strain energy, in bi-axial stress system reaches the limiting distortion energy per unit volume.

\[ \sqrt{\sigma_{n1}^2 + \sigma_{n2}^2 - \sigma_{n1}\sigma_{n2}} = \frac{\sigma_{uu}}{N} \]

Figure: Developed thermal stress distribution at detonation Mach no. 3
Maximum Distortion Energy Theory

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Figure: Developed thermal stress distribution at detonation Mach no. 5

(a) 50 µ (b) 100 µ (c) 150 µ
Maximum Distortion Energy Theory

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Figure: Developed thermal stress distribution at detonation Mach no. 7

(a) 50 $\mu$
(b) 100 $\mu$
(c) 150 $\mu$

Figure: Developed thermal stress distribution at detonation Mach no. 7
Maximum Strain Energy Theory

This theory was developed by Haigh. According to the theory, the failure or yielding occurs at a point in member when the strain energy per unit volume in bi-axial stress system reaches the limiting strain energy per unit volume.

\[
\sqrt{\sigma_{n1}^2 + \sigma_{n2}^2 - 2\nu\sigma_{n1}\sigma_{n2}} \geq \frac{\sigma_{uu}}{N}
\]

(a) 50 \(\mu\)  \hspace{1cm} (b) 100 \(\mu\)  \hspace{1cm} (c) 150 \(\mu\)

**Figure:** Developed thermal stress distribution at detonation Mach no. 3
Maximum Strain Energy Theory

Figure: Developed thermal stress distribution at detonation Mach no. 5

(a) 50 µ  (b) 100 µ  (c) 150 µ
**Maximum Strain Energy Theory**

(a) 50 \( \mu \)  
(b) 100 \( \mu \)  
(c) 150 \( \mu \)

**Figure**: Developed thermal stress distribution at detonation Mach no. 7
Comments on failure theory

(a) Rankine’s Theory  (b) Saint Venant’s Theory  (c) Guest’s Theory
(d) Henckey’s Theory  (e) Haigh’s Theory

Figure: Comparision of failure theories for 50 µm size coal particle at $M = 3$
Observations

- Coal particles subjected to a detonation wave experience highly stressed and strained inner and outer regions.
- Three different regimes emerge in coal particle based on the different particle sizes since the coal particle is subjected to temperature shock.
- The largest particles observed exploded into smaller fragments as break up develops throughout the coal particle. The medium particles observed fragmented in the outer region and left over surviving fraction of same particles are then fragment in the interior.
- The smallest particles observed being fragmented in the interior.
- As the Mack number increases the entire process rapidly speeds up.
- This observations suggest that coal particle under the effect of detonation wave is highly stressed and strained.
- This suggests that detonation combustion of coal is qualitatively different from conventional coal combustion.
**Table:** Time and location where developed thermal stress and strain reaches peak value

<table>
<thead>
<tr>
<th>Mach No.</th>
<th>Size μm</th>
<th>Exposure time $10^{-3}$ secs</th>
<th>Location</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td></td>
<td>1.38</td>
<td>0.1</td>
</tr>
<tr>
<td>5</td>
<td>50</td>
<td>1.38</td>
<td>0.1</td>
</tr>
<tr>
<td>7</td>
<td></td>
<td>All the time</td>
<td>Throughout</td>
</tr>
<tr>
<td>3</td>
<td></td>
<td>2.76</td>
<td>0.1</td>
</tr>
<tr>
<td>5</td>
<td>100</td>
<td>4.41 and 0.85</td>
<td>0.1 and 0.95</td>
</tr>
<tr>
<td>7</td>
<td></td>
<td>All the time</td>
<td>Throughout</td>
</tr>
<tr>
<td>3</td>
<td></td>
<td>2 and 8.82</td>
<td>0.95 and 0.1</td>
</tr>
<tr>
<td>5</td>
<td>150</td>
<td>All the time</td>
<td>Throughout</td>
</tr>
<tr>
<td>7</td>
<td></td>
<td>All the time</td>
<td>Throughout</td>
</tr>
</tbody>
</table>
Theory and Governing Equations: HTM and SMM

Governing heat transfer equation is

\[
\frac{1}{r^2} \frac{\partial}{\partial r} \left( kr^2 \frac{\partial T(r, t)}{\partial r} \right) = \rho C_p \frac{\partial T(r, t)}{\partial t}
\]

Radial and Tangential stresses are given by

\[
\sigma_r = \frac{2\beta E}{(1-\nu)} \left[ \frac{1}{r_0^3} \int_0^{r_0} Tr^2 dr - \frac{1}{r^3} \int_0^r Tr^2 dr \right]
\]

\[
\sigma_t = \frac{\beta E}{(1-\nu)} \left[ \frac{2}{r_0^3} \int_0^{r_0} Tr^3 dr + \frac{1}{r^3} \int_0^r Tr^2 dr - T \right]
\]
Equations governing volatilization are

\[ \frac{\partial V}{\partial t} = -k_0 \exp \left( \frac{-E_a}{RT} \right) (V^* - V)^n \]

\[ \frac{\partial}{\partial r} (Nr^2) = -r^2 \frac{\rho_c}{M_{vol}} \frac{\partial V}{\partial t} \]

Where

\[ N = \frac{r_{pore}^2 \rho \varepsilon}{8 \mu \tau_t R_g T} \frac{\partial p}{\partial r} \]

Total radial stress is given by

\[ \sigma_{r,tot} = p - p_s + \sigma_r \]
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Conditions behind Detonation

Rankine Hugoniot relations used to calculate conditions behind shock wave

\[
\begin{align*}
\frac{T_2}{T_1} &= \frac{2\gamma M^2 - (\gamma - 1) \left[(\gamma - 1)M^2 + 2\right]}{(\gamma + 1)^2 M^2} \\
p_2 &= \frac{2\gamma M^2 - (\gamma - 1)}{p_1} \\
&= \frac{2\gamma M^2 - (\gamma - 1)}{(\gamma + 1)}
\end{align*}
\]
Boundary and Initial Conditions

Boundary conditions are:

\[-k \frac{\partial T}{\partial r} \bigg|_{r=r_0} = h(T - T_\infty) + \sigma_b \epsilon_b (T^4 - T_\infty^4)\]

\[\frac{\partial T}{\partial r} \bigg|_{r=0} = 0\]

\[p \big|_{r=r_0} = p_s\]

And initial conditions are:

\[T(r, 0) = T_{init}\]

\[p \big|_{t=0} = p_s = p_{init}\]
Principal stresses are the eigenvalues of the stress tensor

\[
\bar{\sigma} = \begin{bmatrix}
\tau_{rr} & \tau_{r\theta} & \tau_{r\phi} \\
\tau_{\theta r} & \tau_{\theta\theta} & \tau_{\theta\phi} \\
\tau_{\phi r} & \tau_{\phi\theta} & \tau_{\phi\phi}
\end{bmatrix}
\]
Weibull’s Weakest Link Theory and Fracture Criteria: FCM

- Sequence of events or objects depend on the support of the whole.
- The whole is only as reliable as the weakest member or link.
- The basic assumption for the model is that all materials contain inhomogeneities which are distributed at random.
- When the defects become the fracture origin, it is found that failure is triggered by the largest defect present or, in other words, weakest element present.
- It is possible to indicate a definite probability of the rupture occurring at a given stress or at given time.

Three parameter Weibull’s failure probability is given by

\[ P_f = 1 - e^{-\int \left( \frac{\sigma - \sigma_u}{\sigma_o} \right)^m dV} \]

And fracture criteria is set to

\[ R_f = R_i \text{ for } \Delta P_{f,i} = \max_i \Delta P_{f,i} \text{ and } P_{f,i}^n, P_{f,i}^n \geq P_{f,b} \]
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Comparison Between Analytical and Numerical Solutions

![Graph showing temperature distribution over dimensionless radius]

- **M=3, Numerical Without Radiation, time=1.38 ms**
- **M=3, Numerical With Radiation, time=1.38 ms**
- **M=3, Analytical Without Radiation, time=1.38 ms**
Radial Stress Profile

Radial Stress in N/m²

Dimensionless Radius

Time

Radial Stress Profile

Time

Radial Stress Profile
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Evolution of Tangential Stress Profile

Dimensionless Radius

Tangential Stress Profile

Tangential Stress in N/m²

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Principal Stresses

Figure: Principal stresses at $M = 5$
Volatilization Plots

(a) Volatile Generation

(b) Flow of Volatile

(c) Volatile Pressure

Figure: Volatile matter plots at $M = 4$
Figure: Comparision of $\sigma_r$ with and without volatilization at $M=8$
Effect of Probability

Figure: Local failure probability at $M = 7$
**Effect of Probability**

**Figure:** Comparison of failure probability for different initial volatile matter content at $M = 4$
<table>
<thead>
<tr>
<th>Mach No</th>
<th>Detonation Temperature</th>
<th>Fracture Time</th>
<th>Fracture Temperature</th>
<th>Fracture Location</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>0827.07</td>
<td>7.48420e-04</td>
<td>316.77</td>
<td>0.34</td>
</tr>
<tr>
<td>4</td>
<td>1256.88</td>
<td>8.87846e-05</td>
<td>494.08</td>
<td>0.99</td>
</tr>
<tr>
<td>5</td>
<td>1807.77</td>
<td>3.45506e-05</td>
<td>481.68</td>
<td>0.99</td>
</tr>
<tr>
<td>6</td>
<td>2480.42</td>
<td>1.81286e-05</td>
<td>478.59</td>
<td>0.99</td>
</tr>
<tr>
<td>7</td>
<td>3275.07</td>
<td>1.08422e-05</td>
<td>478.48</td>
<td>0.99</td>
</tr>
<tr>
<td>8</td>
<td>4191.81</td>
<td>6.88620e-06</td>
<td>479.95</td>
<td>0.99</td>
</tr>
</tbody>
</table>
Conclusions

- Numerical solution obtained is compared with analytical solution and it matches with minimum error.
- There is no temperature difference of the numerical solution with and without radiation and hence can be concluded that effect of radiation is negligible.
- Volatilization does not have significant effect on radial stress for the particle size studied here.
- Particle takes longer time to fragment in the interior when subjected to lower Mach number \((M=3)\).
- It takes shorter time for particle to fragment in the surface region when subjected to higher Mach number \((M > 3)\).
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Table: Typical particle size distribution

<table>
<thead>
<tr>
<th>Particle size in µm</th>
<th>Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 to 50</td>
<td>7.5 %</td>
</tr>
<tr>
<td>50 to 90</td>
<td>18.6 %</td>
</tr>
<tr>
<td>90 to 200</td>
<td>31.4 %</td>
</tr>
<tr>
<td>200 to 500</td>
<td>25.1 %</td>
</tr>
<tr>
<td>&gt; 500</td>
<td>17.3 %</td>
</tr>
</tbody>
</table>

- 4 m long detonation tube constructed
- Travel time for $M = 3$ is 3813 µs $M = 8$ is 1429.9 µs.
- Desirable if particle fractures before detonation travel time.

$$\text{Travel Time} = \frac{4}{3\sqrt{\gamma RT}} = \frac{4}{3\sqrt{1.42 \times 287 \times 300}} = 0.003813 \text{ s}$$
PDF for normal distribution is given by

\[ f(x) = \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \]

and CDF is

\[ \phi(x) = \frac{1}{\sigma \sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \, dx \]
Table: Statistical data derived from fracture time for mixture of coal particle subjected to detonation waves of Mach \( nu=6 \)

<table>
<thead>
<tr>
<th>Radius</th>
<th>Fracture Time</th>
<th>Avg. Time</th>
<th>Variance</th>
<th>PDF</th>
<th>CDF</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>5.07e-06</td>
<td>8.0375e-05</td>
<td>1.0993e-04</td>
<td>2.8700e+03</td>
<td>0.2467</td>
</tr>
<tr>
<td>10</td>
<td>4.96e-06</td>
<td>8.0375e-05</td>
<td>1.0993e-04</td>
<td>2.8681e+03</td>
<td>0.2464</td>
</tr>
<tr>
<td>25</td>
<td>6.56e-06</td>
<td>8.0375e-05</td>
<td>1.0993e-04</td>
<td>2.8966e+03</td>
<td>0.2510</td>
</tr>
<tr>
<td>50</td>
<td>1.04e-05</td>
<td>8.0375e-05</td>
<td>1.0993e-04</td>
<td>2.9635e+03</td>
<td>0.2622</td>
</tr>
<tr>
<td>75</td>
<td>1.48e-05</td>
<td>8.0375e-05</td>
<td>1.0993e-04</td>
<td>3.0375e+03</td>
<td>0.2754</td>
</tr>
<tr>
<td>100</td>
<td>1.96e-05</td>
<td>8.0375e-05</td>
<td>1.0993e-04</td>
<td>3.1147e+03</td>
<td>0.2902</td>
</tr>
<tr>
<td>150</td>
<td>3.02e-05</td>
<td>8.0375e-05</td>
<td>1.0993e-04</td>
<td>3.2700e+03</td>
<td>0.3240</td>
</tr>
<tr>
<td>200</td>
<td>4.22e-05</td>
<td>8.0375e-05</td>
<td>1.0993e-04</td>
<td>3.4166e+03</td>
<td>0.3642</td>
</tr>
<tr>
<td>250</td>
<td>5.53e-05</td>
<td>8.0375e-05</td>
<td>1.0993e-04</td>
<td>3.5358e+03</td>
<td>0.4098</td>
</tr>
<tr>
<td>500</td>
<td>1.34e-04</td>
<td>8.0375e-05</td>
<td>1.0993e-04</td>
<td>3.2219e+03</td>
<td>0.6872</td>
</tr>
<tr>
<td>750</td>
<td>2.34e-04</td>
<td>8.0375e-05</td>
<td>1.0993e-04</td>
<td>1.3669e+03</td>
<td>0.9189</td>
</tr>
<tr>
<td>1000</td>
<td>3.49e-04</td>
<td>8.0375e-05</td>
<td>1.0993e-04</td>
<td>1.8332e+02</td>
<td>0.9927</td>
</tr>
</tbody>
</table>
PDF and CDF for time

(a) PDF

(b) CDF

Figure: PDF and CDF plots for fracture time
# Volatile matter statistics

## Table: Volatile matter generation statistics

<table>
<thead>
<tr>
<th>size</th>
<th>Volatile at Fracture</th>
<th>Average Volatile</th>
<th>Volatile Variance</th>
<th>PDF</th>
<th>CDF</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>3.8060e-15</td>
<td>3.3350e-11</td>
<td>4.6522e-11</td>
<td>6.6326e+09</td>
<td>0.2368</td>
</tr>
<tr>
<td>10</td>
<td>5.0426e-12</td>
<td>3.3350e-11</td>
<td>4.6522e-11</td>
<td>7.1262e+09</td>
<td>0.2714</td>
</tr>
<tr>
<td>25</td>
<td>3.2238e-12</td>
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PDF and CDF plots of volatile matter generated at fracture for $M = 6$
Flow of volatile statistics

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PDF and CDF for flow of volatile generation

Figure: PDF and CDF plots of volatile matter flow at fracture for $M = 6$
• Journals

• Conferences and Symposia
Thank You!