# A POCKET MODEL WITH A TETRAHEDRAL CELL FOR ALUMINUM AGGLOMERATION IN COMPOSITE PROPELLANTS

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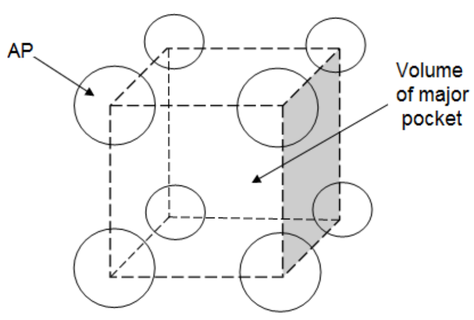
**Aims of the work:**

1. Development of a new model for estimating the size of metal agglomerates.
2. Comparing results of calculations with experimental data and other empirical correlations and models.

## Cohen pocket model




Cohen pocket model

Simplifications of the Cohen model:
1) a regular cubic cell of oxidizer particles;
2) particles of the oxidizer and metal are monodisperse.

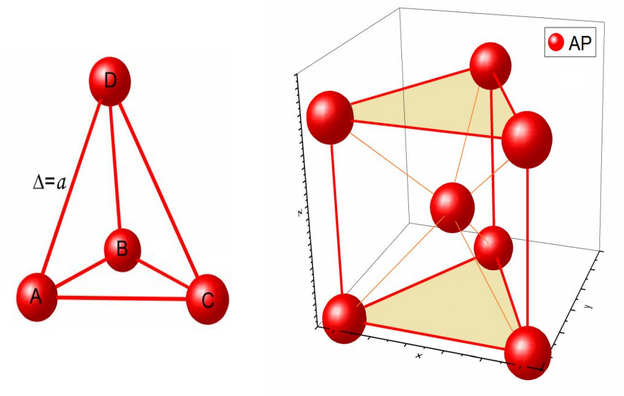
## The calculation of Cohen pocket model

The calculation starts with the largest fraction. For each fraction, we calculated the number of particles per unit volume $N$, the distance between particles $\Delta$, the volume of the pocket $V$, and the size of agglomerate $D_{agg}$.

$$N = \frac{\frac{6\cdot\alpha_{AP}}{\pi\cdot D_{AP}^3}}{\alpha_{AP}\cdot\left(\frac{\rho_{ox}}{\rho_{AP}}\right)+\alpha_{Me}\cdot\left(\frac{\rho_{ox}}{\rho_{Me}}\right)+\alpha_{f}\cdot\left(\frac{\rho_{ox}}{\rho_{f}}\right)} \qquad \Delta = \frac{1-N^{1/3}\cdot D_{AP}}{N^{1/3}} \qquad V_p = \left(\Delta + D_{AP}\right)^3 - \frac{\pi}{6}\cdot D_{AP}^3 \qquad D_{agg} = \left(6/\pi\right)^{1/3}\cdot\left(\gamma\cdot\alpha_{Me}\cdot V_p\right)^{1/3}$$

where $N$ is the number of large particles per unit volume of propellant; $D_{AP}$ is the average size of the oxidizer; $\alpha_{AP}$, $\alpha_f$, $\alpha_{Me}$ are the mass fraction of oxidizer, binder and metal in the propellant; $\rho_{ox}$, $\rho_f$, $\rho_{Me}$ are the density of the oxidizer, binder and metal; $\Delta$ is the distance between AP particles; $V_p$ is effective pocket volume; $D_{agg}$ is the agglomerate size; $\gamma$ is the proportion of molten metal.

## A tetrahedral pocket model




Estimated propellant structure

## The calculation of a tetrahedral pocket model

The calculation begins with the determination of the volume fractions of the components: $\beta_i = \frac{\alpha_i\cdot\rho}{\rho_i}$

The iteration method is used to select the distance ***a*** between the centers of AP particles so that the volume fraction of AP in the triangular prism corresponds to the specified volume fraction of AP in the propellant

$$\beta'_{AP} = \frac{V_{AP}}{V_{prism}} = \frac{\pi\cdot D_{AP}^3}{2\sqrt{2}\cdot a^3}$$

Volume of pocket: $V_{pocket} = V_{tetr} - 4V_{tetr\ D_{AP}} = \frac{\sqrt{2}}{12}\left(a^3 - \frac{D_{AP}^3}{2}\right)$ Agglomerate size: $D_{agg\ tetr\ mod} = \left(\frac{6\cdot\beta_{Me}\cdot V_{pocket}}{\pi}\right)^{1/3}$

where $\beta_i$, $\alpha_i$, $\rho_i$ are volume fraction, mass fraction and density of the i-th propellant component; $\rho$ is density; $V_{AP}$ is the volume of AP inside the prism; $V_{prism}$ is the volume of the prism; $D_{AP}$ is AP size; $a$ is the distance a between the centers of AP particles; $V_{tetr}$ is the volume of the tetrahedron; $V_{tetr\ DAP}$ is the volume of the tetrahedral parts occupied by AP; $\beta_{Me}$ is the volume fraction of metal in reference propellant binder+Me.

## Comparing results of calculations with experimental data and other empirical correlations and models

### Propellant compositions

| | Propellant 1 | | Propellant 2 | | Propellant 3 | |
|---|---|---|---|---|---|---|
| **Component** | α | $D_{43}$, μm | α | $D_{43}$, μm | α | $D_{43}$, μm |
| **Coarse AP fraction** | 0.37 | 306 | 0.37 | 306 | 0.41 | 301 |
| **Fine AP fraction** | 0.27 | 17.1 | 0.15 | 17.1 | 0.21 | 13.1 |
| **Binder** | 0.18 | – | 0.30 | – | 0.20 | – |
| **Aluminum** | 0.18 | 29.2 | 0.18 | 29.2 | 0.18 | 15.2 |
| **Agglomerate size (exp.) $D_{43}$, μm** | 669 | | 187 | | 179 | |
| **Burning rate, mm/s** | 11.5 ($p$ = 4.3 MPa) | | 15.2 ($p$ = 4.4 MPa) | | 39 ($p$ = 4.9 MPa) | |

### Empirical correlations and models of agglomerates

Hermsen correlation

$$D_{Hermsen} = \frac{907.4}{r_b\cdot Y_{AP}}$$

Salita correlation

$$D_{Salita} = \frac{869}{r_b\cdot\left(Y_{AP}+Y_{Al}\right)^2}$$

Beckstead correlation

$$D_{Beckstead} = \frac{1}{2}\left(\frac{\xi_{Al}}{\xi_{AP,C}}\right)^{1/3} D_{AP,C}$$

Cohen pocket model

$$D_{Cohen} = \left(\frac{\rho_{Al}Y_{Al}}{\rho_{AP}Y_{AP,C}}\right)^{1/3} D_{AP,C}$$

Grigoriev correlation

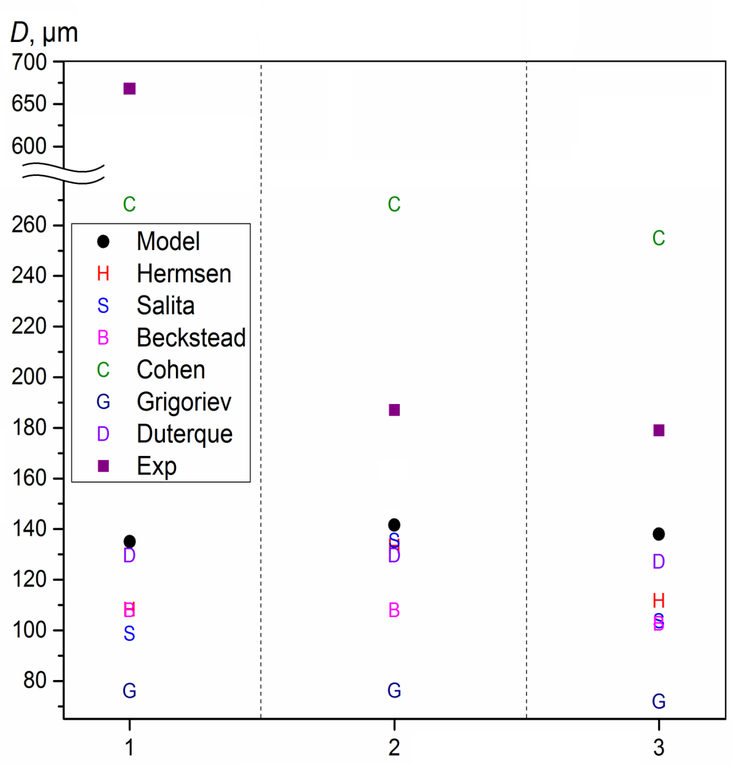
$$D_{Grigoriev} = \frac{2}{3}\xi_{Al}^{1/3}\left(1-\xi_{AP,C}\right)^{2/3} D_{AP,C}$$

Duterque correlation

$$D_{Duterque} = 2.42\frac{D_{Cohen}}{r_b} + 80.26$$

$D$ Is AP particle size, μm; AP is the total AP fraction; AP,C is coarse fraction of AP; $Y$ is the mass fraction of the component; ξ is the volume fraction of the component; $r_b$ is burning rate, mm/s.

### Size of aluminum agglomerates




## Conclusion

- A new simplified tetrahedral pocket model has been developed for estimating the size of metal agglomerates during the combustion of a solid propellant.
- It is shown that, it is impossible to carry out calculations for the propellant containing 0.65 AP, 0.15 binder and 0.2 aluminum using the Cohen model. For this propellant, the distance between particles takes on a negative value Δ = – 2.8 μm, and the structure of such propellant does not correspond to cubic packing. The proposed tetrahedral model (Δ = 88 μm) makes it possible to carry out calculations for propellants for which the Cohen model does not provide a solution.
- The experimental data are compared with the results of calculations using the tetrahedral model, the Cohen model, and the empirical correlations of Hermsen, Salita, Beckstead, Grigoriev, Duterque.
- It is shown that the proposed tetrahedral pocket model in some cases gives better results for predicting the agglomeration diameter than other models.

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