

# POROUS STRUCTURE EVOLUTION AND FRAGMENTATION OF HIGHLY POROUS CHARs UNDER OXIDATION

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## Introduction

Fragmentation of small coal particles influences the effectiveness of their combustion and pollutant emission, however, its nature is not yet fully understood. The threshold for fragmentation is determined mainly by the porous structure of the coal. Real coals usually have a polymodal pore size distribution. The role of the different modes for bulk fragmentation has not been studied so far. Here, this issue is presented by studying a model material (Spherocharb synthetic char) under both uniform and non-uniform oxidation.

## Porous Structure

The porous structure of char is considered as constructed from randomly oriented interconnected solid micro-crystals (Fig. 1). The skeleton of the microcrystals together with the intercrystal voids (S-pores) form the microstructure. This skeleton is a connected domain, which can be bounded, inside the particle, by large pores (L-pores), with dimensions much larger than the mean dimensions of the microcrystals. This porous structure was modeled by Kantorovich and Bar-Ziv [1].

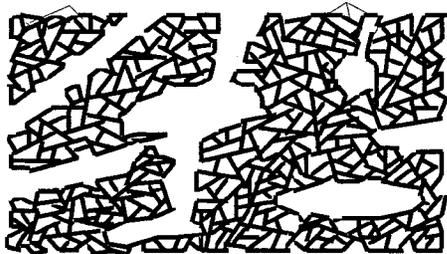


Figure 1. Schematics of the porous structure.

## Pore Size Mode Controlling Fragmentation

The controlling mode of the porous structure was determined from the following considerations:

- 1.No-Fragmentation occurred for carbonaceous materials that undergo shrinking in kinetically controlled conditions (regime I). Spherocharb chars never fragmented under regime I combustion (though the initial porosity of Spherocharb char is close to the

fragmentation threshold predicted and observed for other classes). A distinctive property of this class is shrinkage under regime I conditions.

- 2.The only geometrical property which does not change during conversion of these chars is the L-porosity. Shrinkage can be described by the evolution of the microstructure [1], which includes: (1) preferential consumption and break of intercrystal joints; (2) restoration of the broken joints by attraction forces; (3) change of the microcrystal position and a subsequent formation of new joints; (4) coalescence of the microcrystals to their neighbors. The micro-structure can be considered as the walls of the L-pores, The L-pores follow the change in microstructure dimensions, due to shrinkage. Their volume reduces with the same rate as the volume of the micro-structure, i.e., porosity of the L-pores does not change with conversion. From Fig. 2 one can see that the L-porosity is the only geometrical property that does not change during conversion (internal porosity is the ratio of volume of S-pores to volume of the micro-structure). As fragmentation is a geometrical problem and porosity is among the determining geometrical factors, it is logical to assume that the L-porosity controls fragmentation.

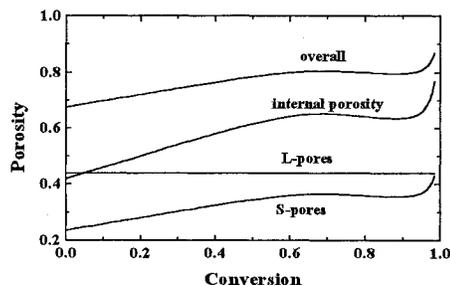


Figure 2. Porosity (different modes) vs. conversion for a uniformly heated particle; model calculation.

trigger the L-porosity by oxidizing these chars in intentionally induced conditions.

## Triggering L-Porosity

L-porosity can be triggered if the reaction rate is non-uniform. In this study we consider two ways of non-uniform reactivity:

1. Local fragmentation under non-uniform heating. If a temperature gradient is induced within the particle, the rate of shrinkage of each portion of the microstructure changes with its position, which causes deformation of internal borders of the microstructure and a non-uniform change in the L-porosity. Figure 3 shows the calculated evolution of L-porosity at different places inside the particle. If maximum L-porosity exceeds the threshold of fragmentation, the particle fragments locally, forming the hole at the center. This is confirmed in experiments on oxidation of a single Spherocarb char particle suspended in the electrodynamic chamber, which was heated from its bottom by laser radiation (see Fig. 4).

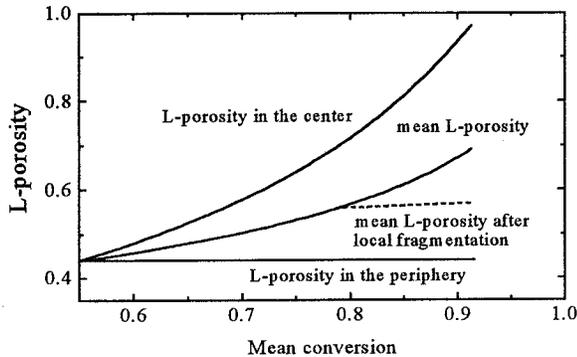


Figure 3. Evolution of L-porosity and mean porosity.

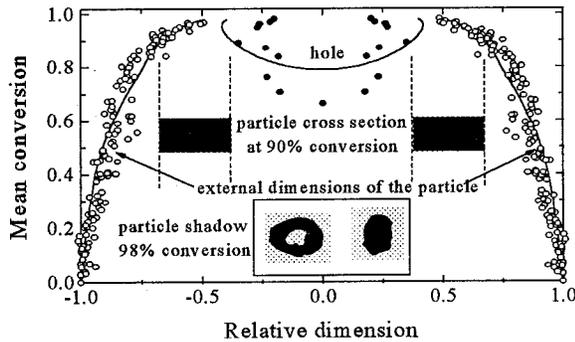


Figure 4. Evolution of external and internal dimensions of a non-uniformly heated particle; open circles - external dimensions, solid circles - hole dimensions, solid line - calculations. A calculated cross section of the particle at 90% conversion is provided and in the inset are shadows of a particle from two perpendicular sides as measured at 98% conversion.

2. Local fragmentation under oxygen concentration gradient. Non-uniformity in reactivity due to non-uniform oxygen concentration occurs under diffusion controlled conditions (regime II). For a spherical char particle it would lead to the maximum of the L-porosity in the periphery and to the peripheral fragmentation, as was indeed observed [2]. This phenomenon is analogous

to the case of non-uniform heating (see. Fig. 5). It supports the controlling role of L-pores in fragmentation.

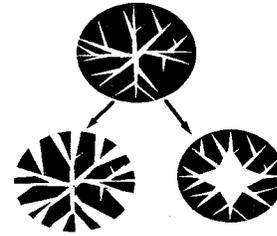


Figure 5. The change in the porous structure for two different cases of non-uniform oxidation.

## Conclusions

Fragmentation of oxidizing char particles is determined by the L-pores with dimensions much larger than the mean dimension of a microcrystal within the micro-skeleton. For Spherocarb char the L-pores include meso- and macro-pores. Non-fragmentation of uniformly oxidizing particles, that undergo shrinkage, is due to unchanged porosity of the L-pores. The reason for the local fragmentation under non-uniform oxidation is the increase in the local macroporosity at a particle's center, due to non-uniform shrinkage of the micromedium.

## Acknowledgments

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## References

1. Kantorovich, I.I., and Bar-Ziv E., *Combustion and Flame*, 1994, 97: 61.
2. Helble, J. J. and Sarofim, A. F., *Combustion and Flame*, 1989, 76:183.