14

Coupling radiative properties with detailed char conversion kinetics

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Motivation

- In pulverized fuel combustion systems, particle radiation is the dominant heat transfer mechanism.
  - Precise description is crucial for predictive simulations.
  - Particle radiation depends strongly on optical particle properties, characterized by the index of refraction – **IOR**
- During conversion of the particle, optical properties change
  - For burnout $B = 0$, IOR of the solid fuel $\boldsymbol{m}_{\mathbf{SF}}$ is known:
    - $\boldsymbol{m}_{\mathbf{SF}} = 1.8 + 0.0713\mathrm{i}$
  - For burnout $B = 1$, IOR of ash $\boldsymbol{m}_{\mathbf{Ash}}$ is known:
    - $\boldsymbol{m}_{\mathbf{Ash}} = 1.5 + 0.0189\mathrm{i}$
- Large-scale CFD simulations apply simplified models to consider the burnout-dependent properties, e.g.:
  - $\boldsymbol{m}_{\mathbf{SF}}$ is used for $0 \le B \le 0.5$
  - $\boldsymbol{m}_{\mathbf{Ash}}$ for $0.5 < B \le 1$

Is this simplified approach sufficiently accurate? or **Is a precise description of the particle radiative properties necessary?**

Coupling Char Conversion Kinetics model to Discrete-Dipole Approximation

- Input
  - Initial particle diameter $D_{\mathrm{Particle},0} = 100\ \mu\mathrm{m}$
  - Proximate analysis (C, H, S, O, N and ash)
  - Gas and particle temperature
  - Oxygen transport within particle pores and boundary layer
  - High volatile bituminous coal was used

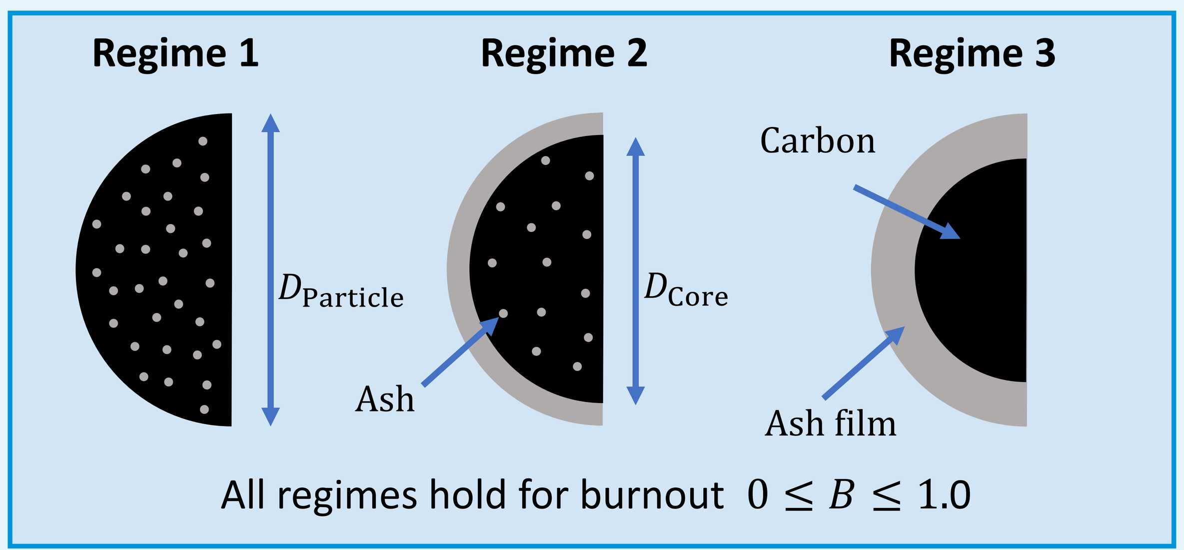


Figure 1: Depending on the oxygen transport, particle reacts in different regimes.

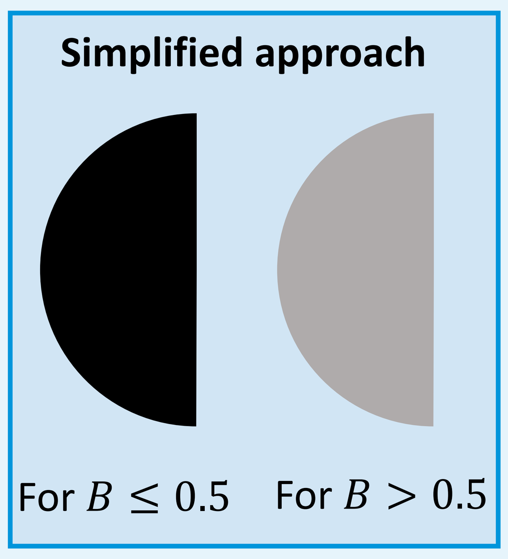
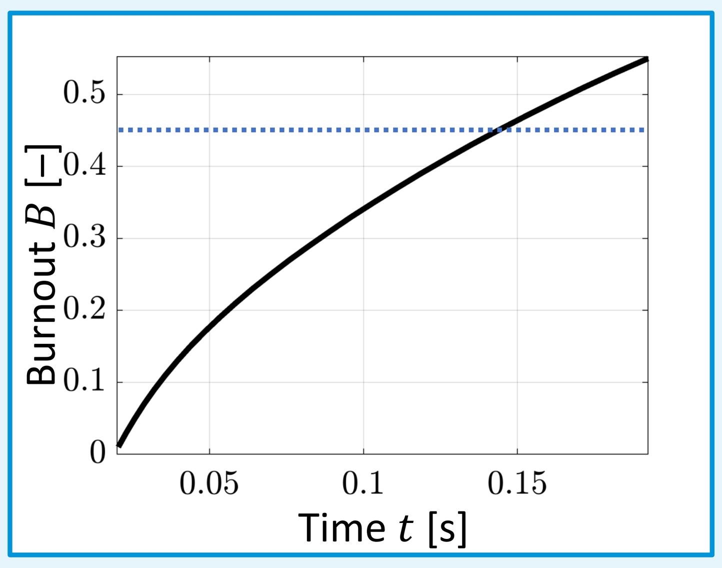
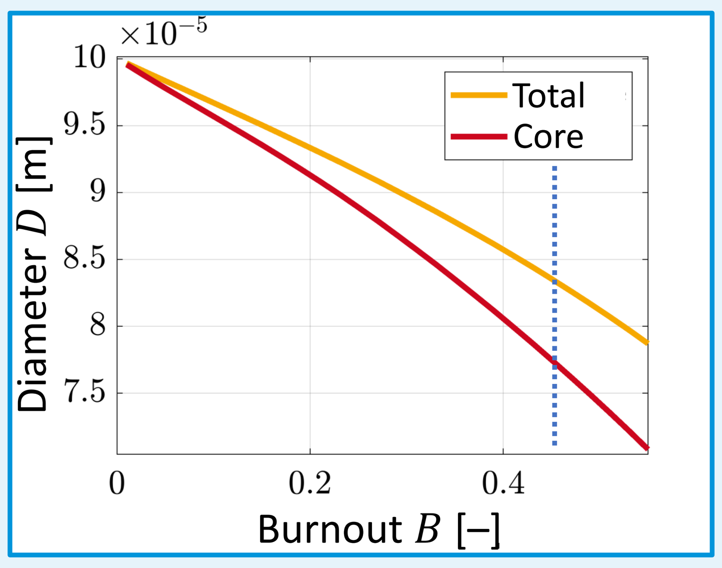


Figure 2: Illustration of a simplified approach

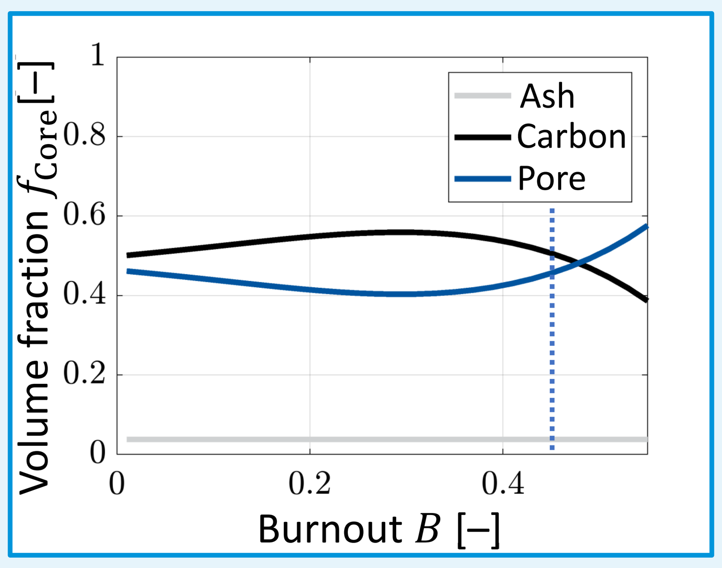
- **Output** for a particle burning **in regime 2**
  - Burnout B



  - Total and core diameter



  - Volume fraction in the core



  - Volume fraction in the ash film

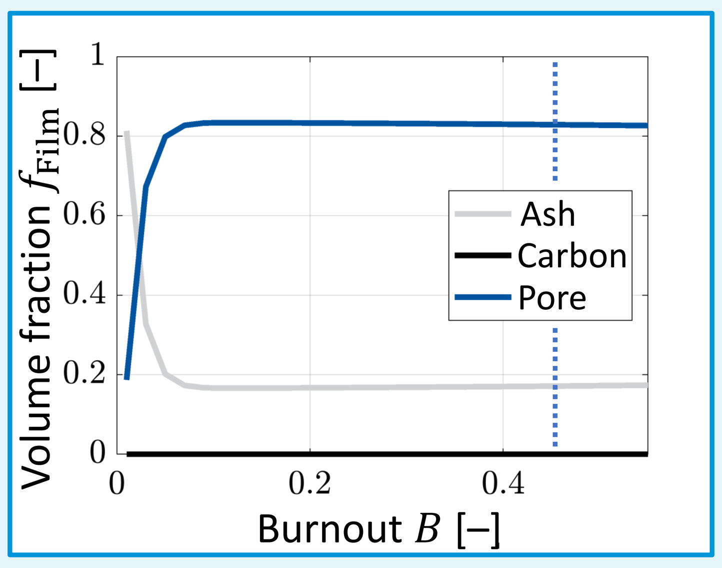


Figure 3: Output for a particle burning in regime 2. For burnout $B > 0.45$ the CCK data was extrapolated (marked by blue dotted line). For regime 1 and 3 the same particle diameter as in regime 2 was used.

- Input
  - Particle diameter D_{Particle} and core diameter D_{Core}
  - Ash, carbon and pore volume fraction of particle
  - IOR of corresponding material
  - Wavelength of interacting radiation

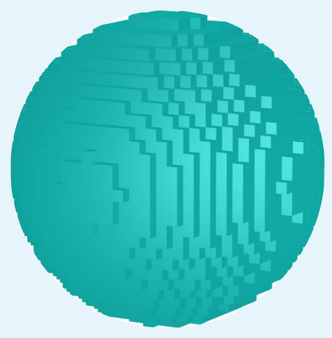
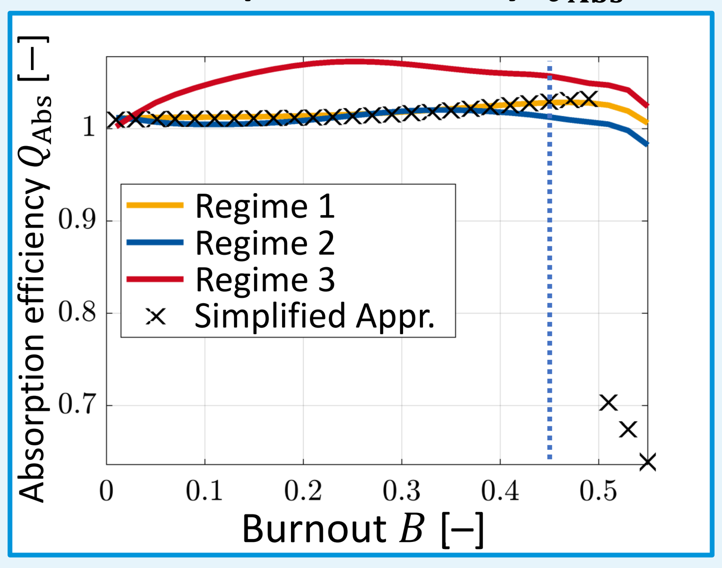


Figure 4: Exemplary DDA mesh

- Output
  - **Absorption efficiency Q_{Abs}**



  - **Scattering efficiency Q_{Sca}**

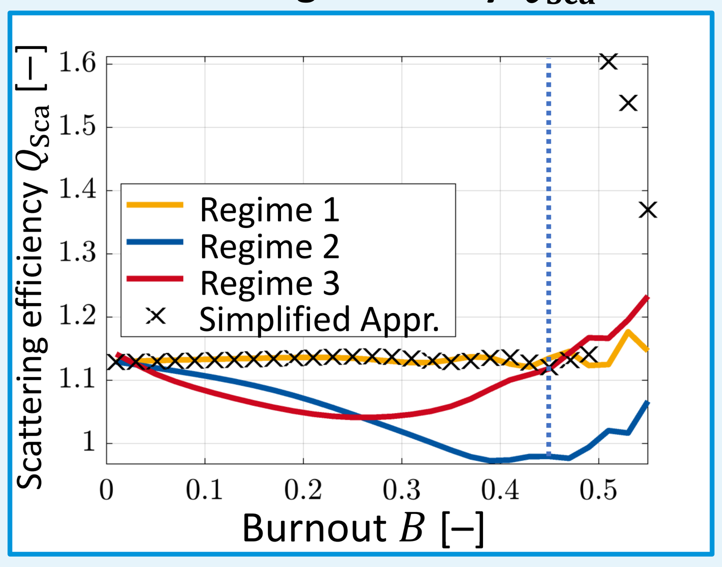


Figure 5: Resulting absorption and scattering efficiency – the dotted line divides between the results obtained applying CCK data and extrapolated CCK data.

  - **Phase function Φ**

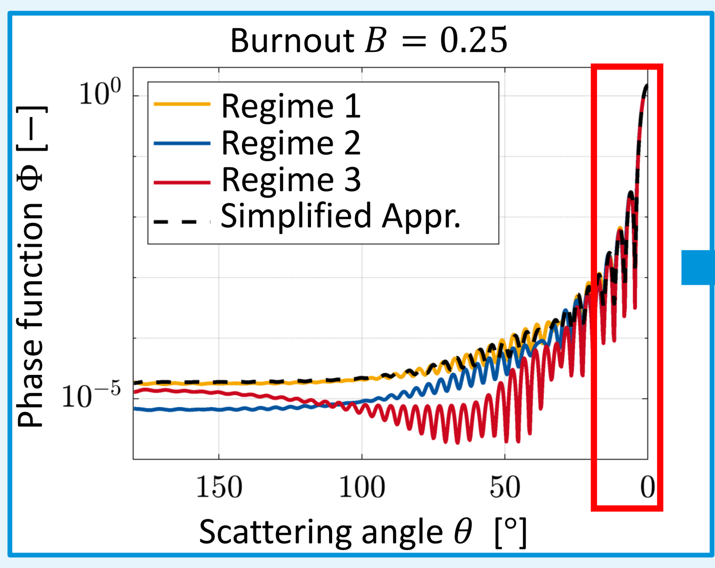


Figure 6: The phase function gives the redistribution of scattered radiation in spatial directions. Forward direction is 0° and backwards is 180°.

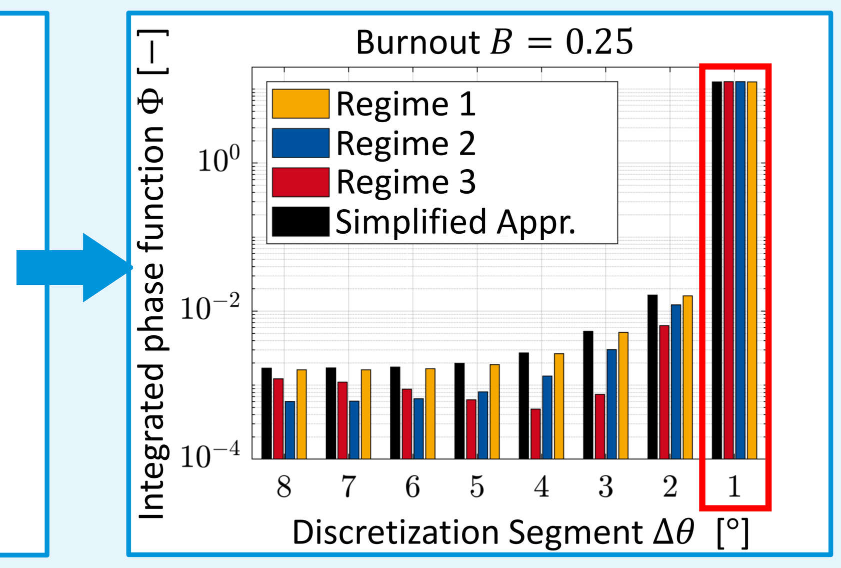
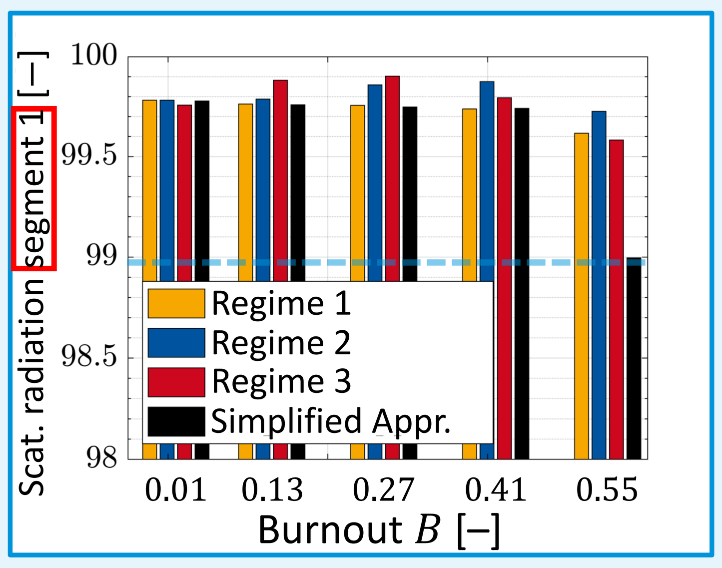


Figure 7: In CFD, a discretized version of Φ is applied. Here, the phase functions is integrated evenly over 8 discretization segments.



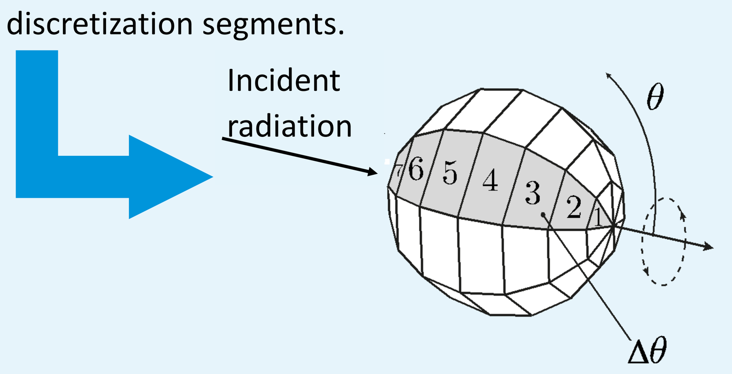


Figure 8: For the investigated particle, 99 % of the scattered radiation is scattered in segment 1. Therefore, it is not necessary to distinguish between the regimes or the simplified approach regarding the phase function. However, the conversion of smaller particles needs to be studied next, as smaller particle indicate distinct sideward scattering.

Conclusion

- The simplified approach is in a good agreement for $B < 0.5$ with the CCK model. Especially the results of regime 1 coincide with the results of the simplified approach. For $0.5 < B < 0.6$ the deviation increases drastically, and thus, the simplified model is not recommended. As the imaginary part of m_{SF} is much larger than m_{Ash}, the influence of m_{SF} on the radiative properties are more distinct even for $0.4 < B < 0.5$.
- The scattering phase function indicates higher deviation for sideward and backward scattering $\theta > 22.5°$. However, as more than 99 % of the scattered radiation is scattered forward in all cases, scattering can be neglected for the investigated particle.
- In future studies, the influence of $0.6 < B < 1.0$ on the radiative properties as well as smaller particles are investigated.
- The advanced model is recommended for the calculation of single particle properties. The impact of this modeling approach on the temperature distribution in a combustion chamber is investigated next.

Acknowledgements

This work has been funded by the German Research Foundation (DFG) – project number 215035359 – within the framework of the CRC/Transregio 129 "Oxyflame".

OXYFLAME

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