# Implementation of reactive particles into Pencil Code DNS

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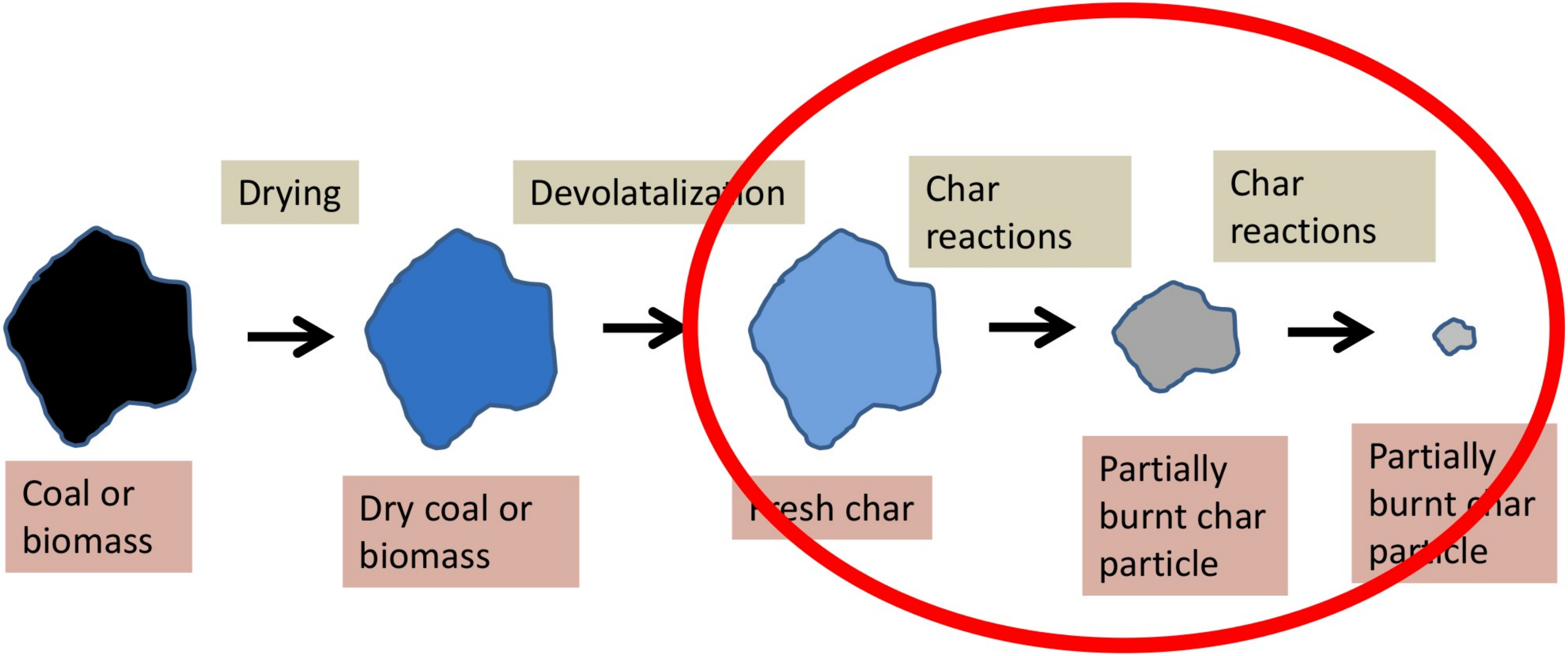
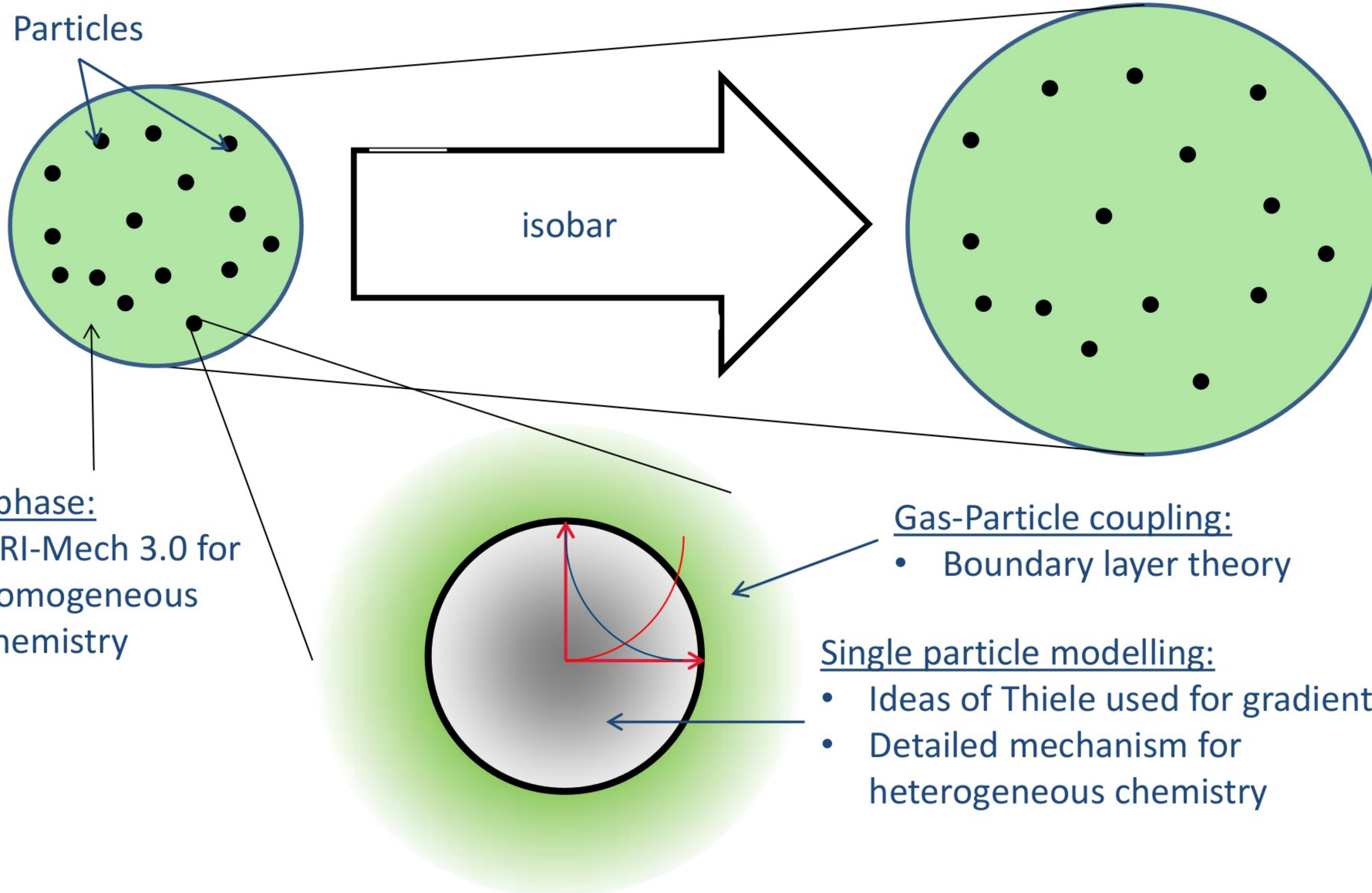
# Solid fuel reactions



# Stand-alone model (or sub model for CFD)




<u>Gas phase:</u>

- GRI-Mech 3.0 for homogeneous chemistry

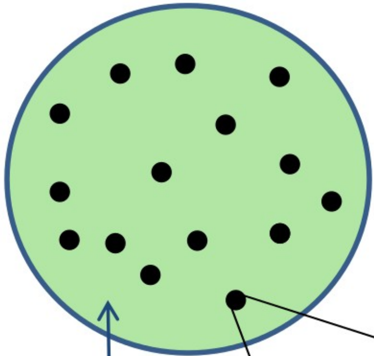
<u>Gas-Particle coupling:</u>

- Boundary layer theory

<u>Single particle modelling:</u>

- Ideas of Thiele used for gradients
- Detailed mechanism for heterogeneous chemistry

# Stand-alone model

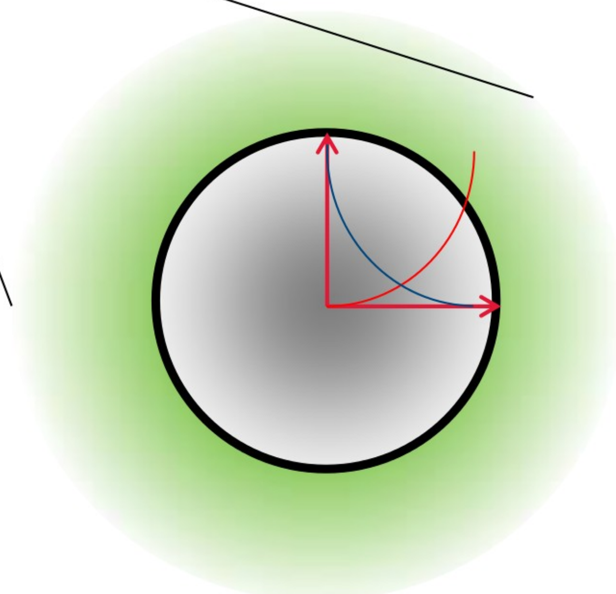


**Gas phase equation:**

1. Temperature
2. Mass
3. Species

**Gas phase:**

- GRI-Mech 3.0 for homogeneous chemistry



**Particle phase equations:**

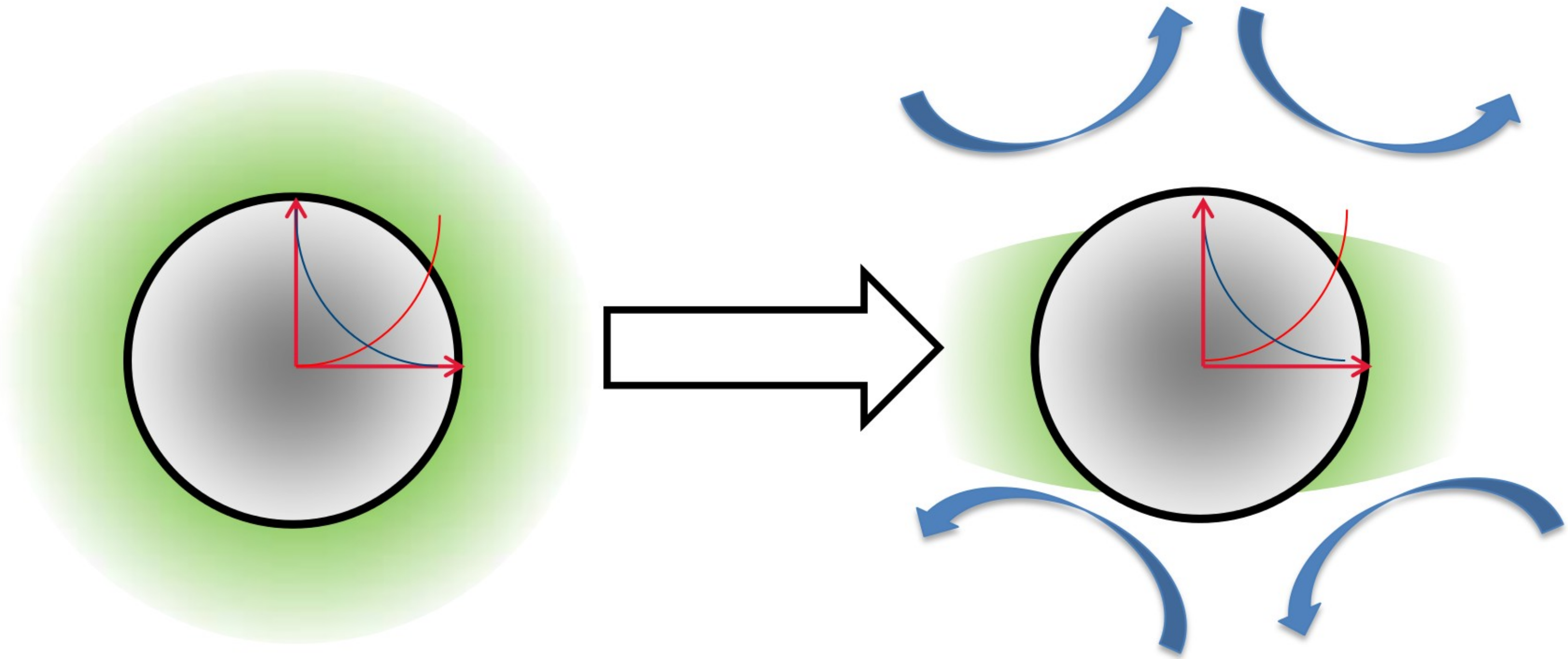
1. Temperature
2. Mass
3. Adsorbed species

# Heterogeneous reaction mechanism

| Nr | Reaction | $A_k$ | $E_k$ | $\sigma_k$ |
|---|---|---|---|---|
| 1 | 2Cf + H2O $\Leftrightarrow C(OH) + C(H)$ | 2.10e12 | 105. | |
| 2 | C(OH) + Cf $\Leftrightarrow C(O) + C(H)$ | 4.10e14 | 80. | |
| 3 | 2C(H) $\Leftrightarrow 2Cf + H2$ | 1.40e14 | 67. | |
| 4 | C(O) $\Rightarrow Cf + CO$ | 1.00e13 | 353. | 28e6 |
| 5 | C(OH) $\Leftrightarrow HCO + Cf$ | 1.00e13 | 393. | 28e6 |
| 6 | Cf + C(H) + H2O $\Leftrightarrow CH3 + C(O) + Cf$ | 1.00e19 | 300. | |
| 7 | Cf + C(H) + H2 $\Leftrightarrow CH3 + 2Cf$ | 1.00e19 | 300. | |
| 8 | Cf + C(H) + CO $\Rightarrow HCO + 2Cf$ | 1.00e19 | 300. | |
| 9 | 2C(H) $\Rightarrow CH2 + Cf$ | 3.00e14 | 426. | |
| 10 | Cf + CO2 $\Leftrightarrow C(O) + CO$ | 3.70e06 | 161. | |
| 11 | C(O) + CO2 $\Rightarrow C(O) + 2CO$ | 1.26e11 | 276. | |
| 12 | Cf + CO $\Leftrightarrow C(CO)$ | 1.00e16 | 455. | 53e6 |
| 13 | CO + C(CO) $\Rightarrow CO2 + 2Cf$ | 9.80e09 | 270. | |
| 14 | 2Cf + O2 $\Rightarrow C(O) + CO$ | 5.00e16 | 150. | |
| 15 | 2Cf + O2 $\Rightarrow C2(O2)$ | 4.00e13 | 93. | |
| 16 | Cf + C(O) + O2 $\Rightarrow CO2 + C(O) + Cf$ | 1.50e13 | 78. | |
| 17 | Cf + C(O) + O2 $\Rightarrow CO + 2C(O)$ | 2.10e13 | 103. | |
| 18 | C2(O2) $\Rightarrow CO2 + 2Cf$ | 1.00e13 | 304. | 33e6 |

Reversible reactions are calculated by using the equilibrium constant

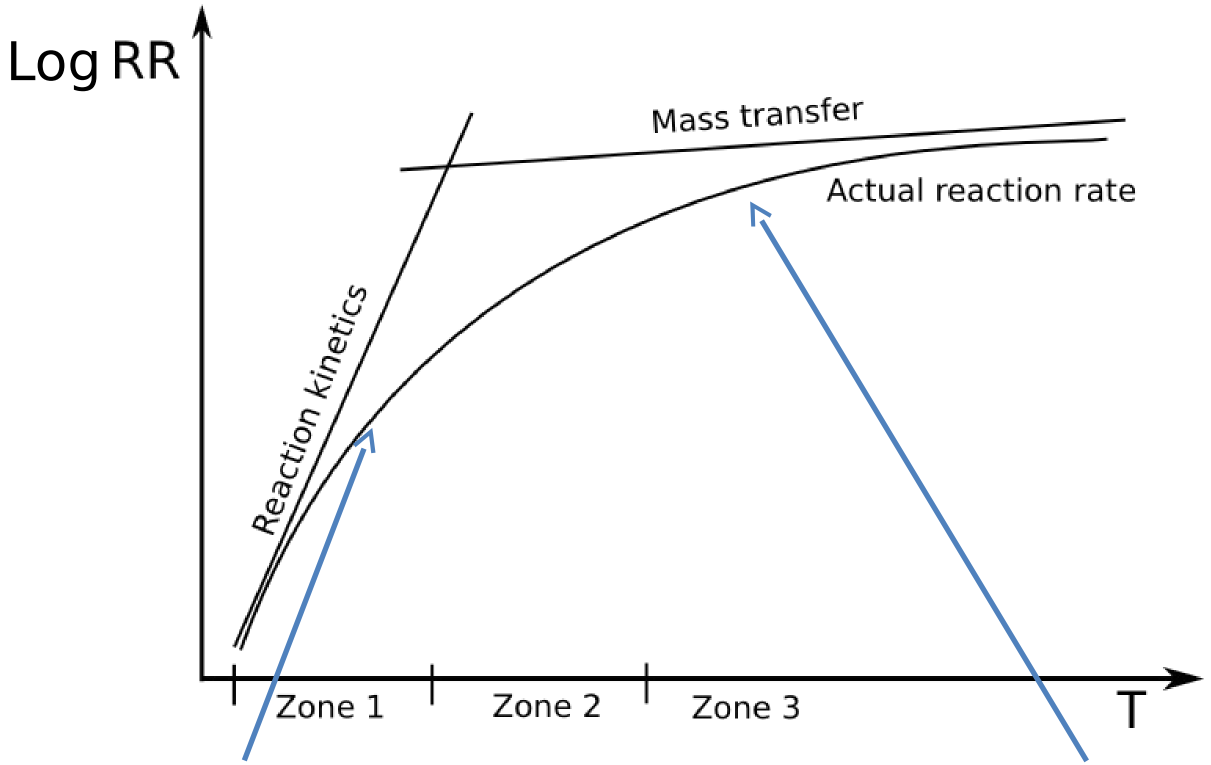
# The project



Quiescent gas, uniform behaviour for all particles

Flow turbulence coupling, behaviour unique for each particle

# Conversion regimes

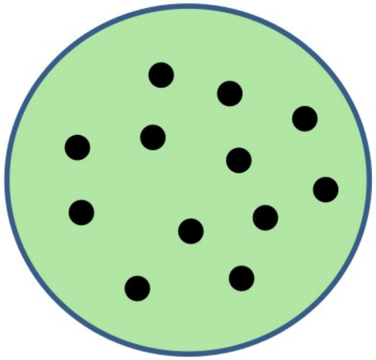



Reactions throughout the particle,
mass loss by decrease in apparent density

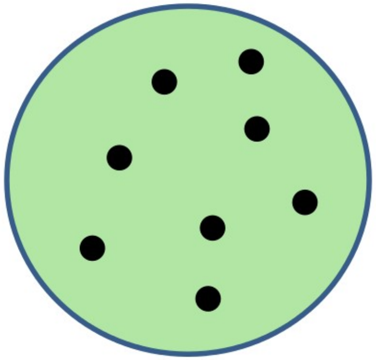
Reactions on the surface,
mass loss due to radius
decrease

# Case simulated in standalone model

| Property | | Case A | Case B |
|---|---|---|---|
| Carbon to gas mass ratio | $m_p/m_g$ | 0.3 | 0.2 |
| Particle number density | $n_p$ | $3.1 \times 10^9$ | $2.1 \times 10^9$ |
| Equivalence ratio | $\phi$ | 2.76 | 1.84 |

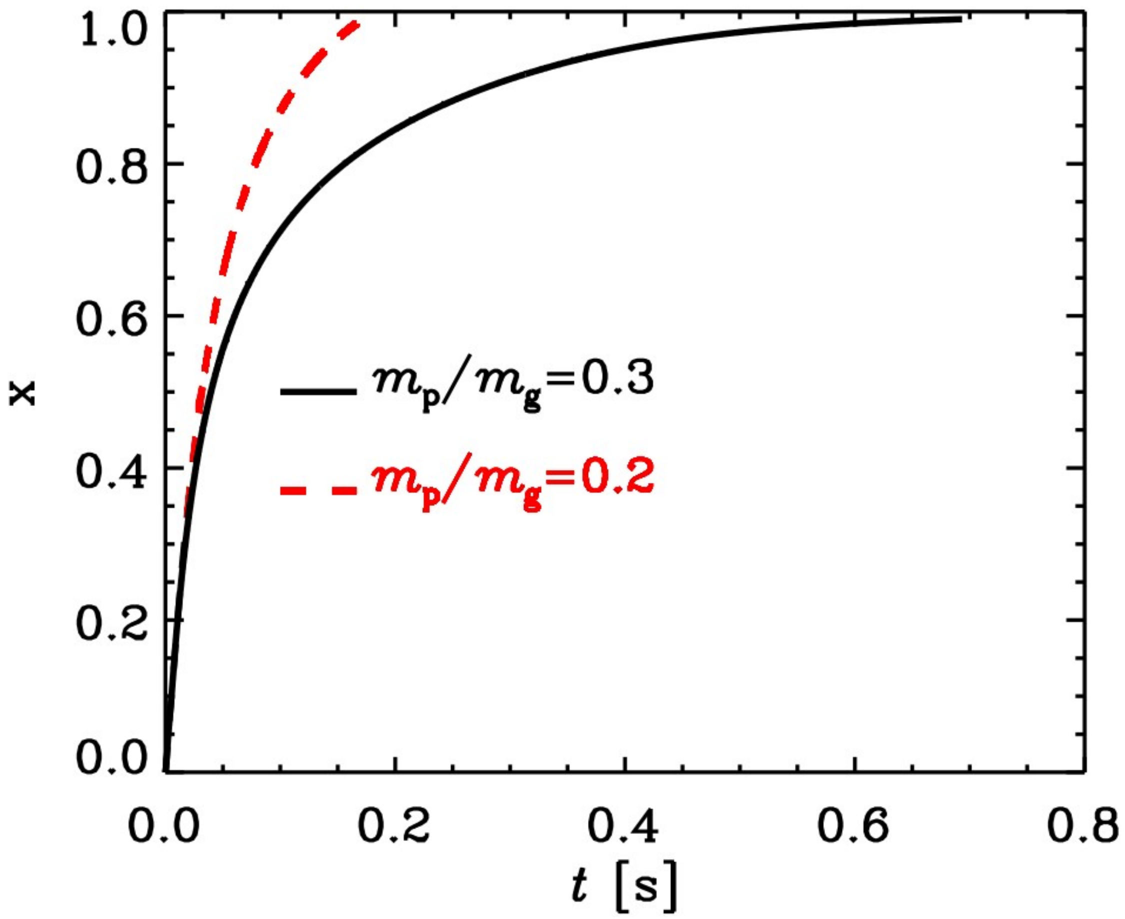


Case A



Case B

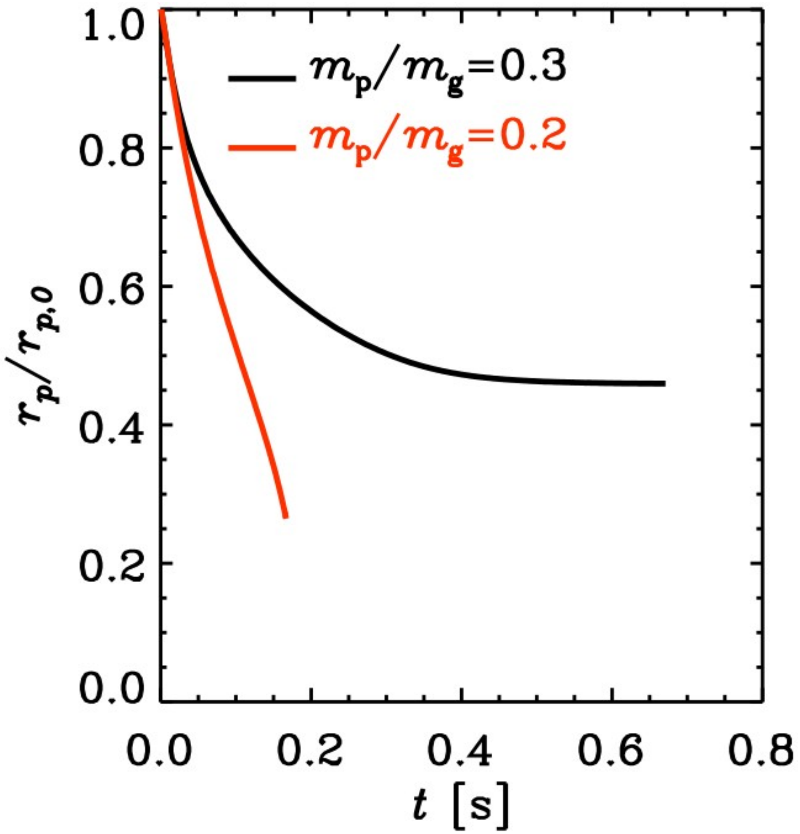
# Results




Particle conversion over time

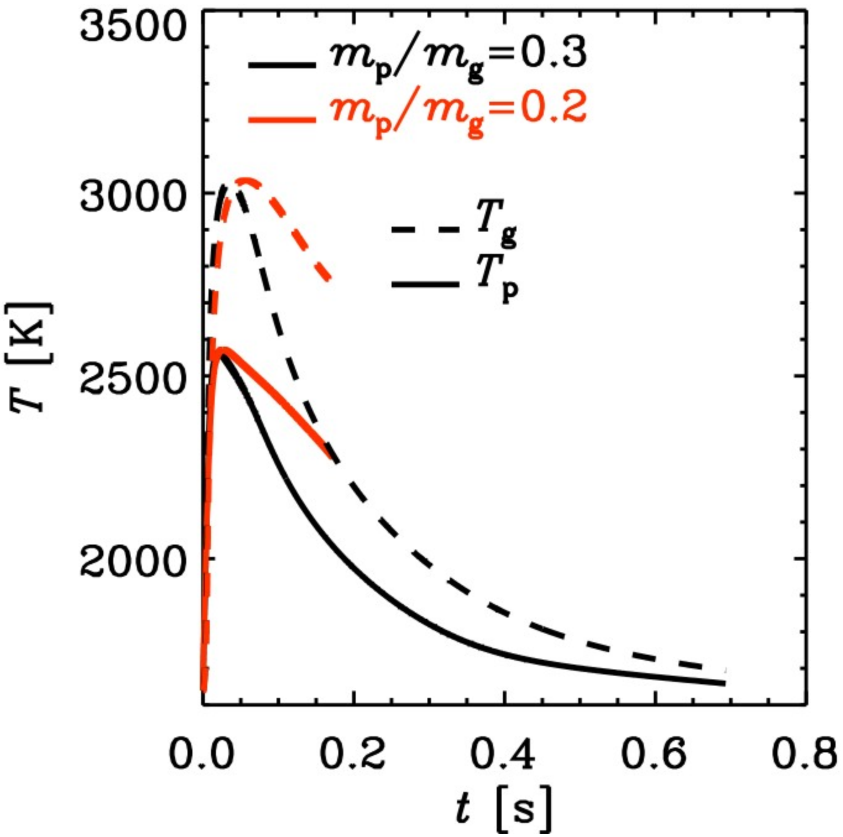
Conversion for smaller load 5x faster

# Results




Particle radius over time

Different modes of conversion




Particle and gas temperature over time

# Adding of source terms into the equations

- Mass

$$\frac{\mathrm{D}\ln\rho}{\mathrm{D}t} = -\nabla\cdot\boldsymbol{u} + S_\rho$$

- Momentum

$$\frac{\mathrm{D}\boldsymbol{u}}{\mathrm{D}t} = \frac{1}{\rho}(-\nabla p + \boldsymbol{F}_{vs}) + \boldsymbol{f} + \boldsymbol{S}_u$$

- Species

$$\rho\frac{\mathrm{D}Y_k}{\mathrm{D}t} = -\nabla\cdot\boldsymbol{J}_k + \dot{\omega}_k + S_{y,k}$$

- Energy

$$\left(c_p - \frac{R}{m}\right)\frac{\mathrm{D}\ln T}{\mathrm{D}t} = \sum_k \frac{\mathrm{D}Y_k}{\mathrm{D}t}\left(\frac{R}{m_k} - \frac{h_k}{T}\right) - \frac{R}{m}\nabla\cdot\boldsymbol{u} + \frac{2\nu\boldsymbol{S}^2}{T} - \frac{\nabla\cdot\mathbf{q}}{\rho T} + q_c + S_T$$

# Roadmap

- Implementation of a model with two-way coupling between particle and gas phase
  - Mass
  - Momentum
  - Species
  - Energy
- Application and verification with DNS

# Questions?

# What we need (preliminary)

- Particle radius module $$\frac{dr_p}{dt} = \begin{cases} 0 & \text{if } t < \tau_c, \\ \frac{dm_p}{dt}\frac{1-\eta}{4\pi r_p^2 \rho_p} & \text{if } t \geq \tau_c. \end{cases}$$
- Particle chemistry
  - Particle mass (together with particle radius will be particle density)
  - Particle temperature
  - Particle adsorbed species
- Source term in momentum equation $$\frac{\mathrm{D}\boldsymbol{u}}{\mathrm{D}t} = \frac{1}{\rho}(-\nabla p + \boldsymbol{F}_{vs}) + \boldsymbol{f} + \boldsymbol{S}_u$$