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Numerical investigation on factors of graphene obtained by chemical vapor deposition

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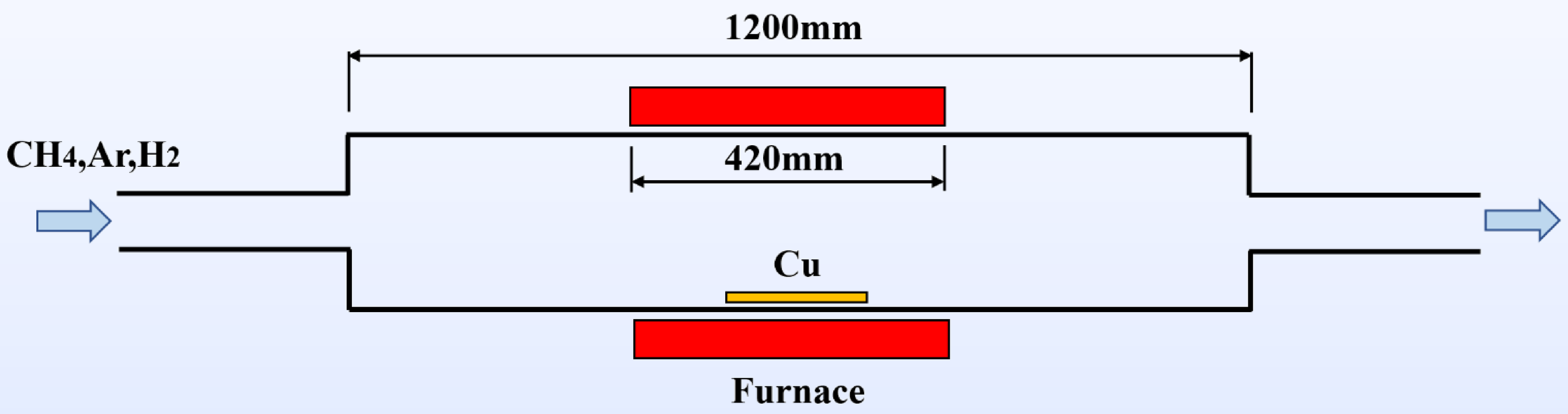
Background

Graphene has received widespread attention because of its superior properties, and chemical vapor deposition is expected to become an ideal method for preparing large-area high-quality graphene. There are many influencing factors for growing graphene by the CVD method, including substrate, carbon source, growth conditions such as gas flow rate, temperature, pressure, deposition time, cooling rate, etc.

Most studies on graphene growth mainly focus on the surface growth mechanism. However, gas-phase process and thermal field control also play an important role in the growth of graphene, especially when the reactor size gradually increases. In this paper, the temperature distribution and flow state in the reactor are calculated by numerical simulation, and the deposition rates at different locations in the reactor are compared.

Modelling

Geometry



Simulation setting

- Species transport model
- Reaction model
- Incompressible ideal gas
- Inlet gas flow rate: 1.35e-5 kg/s
- Furnace temperature: 1025K

$$CH_4 \rightarrow C + 2H_2$$

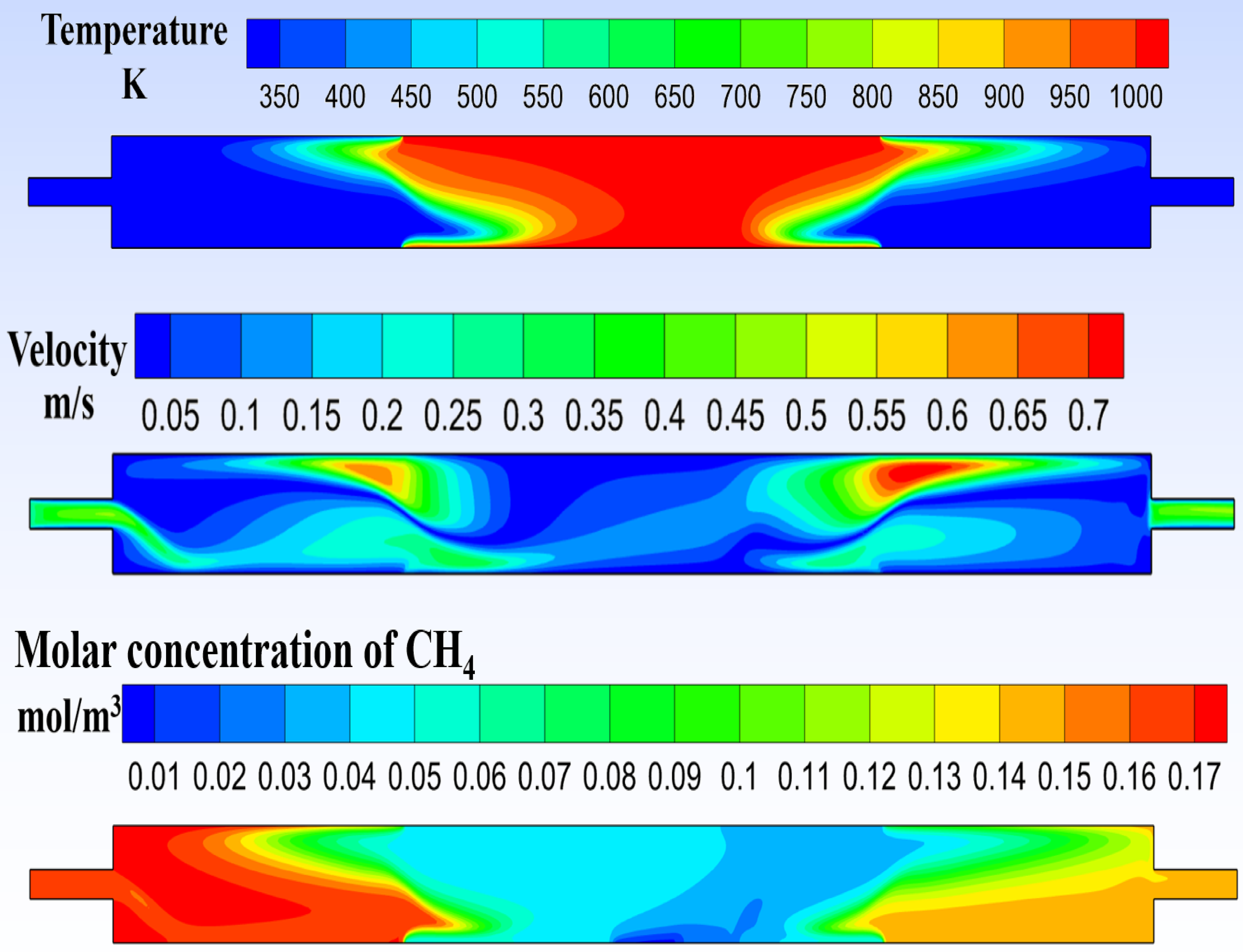
- Effective reaction constant

$$k_s = Ae^{-\frac{E}{RT}}$$

$$A = 10^9 \quad E = 2.5\times10^8$$

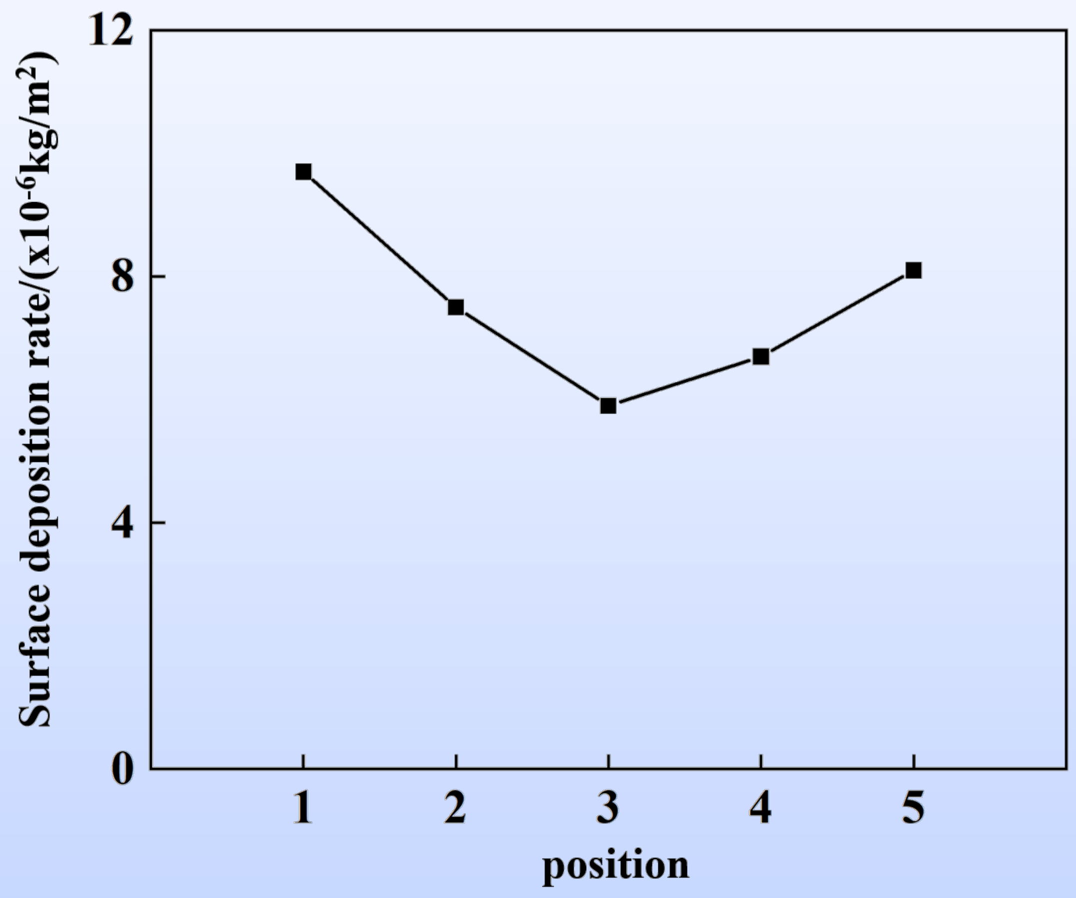
Results

Results

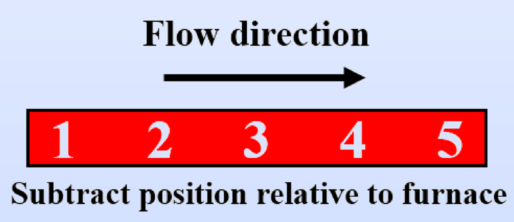


- The temperature and velocity are not uniform near the furnace boundary, which is caused by thermal buoyancy due to relatively large density variations.
- The velocity distribution above the subtract is uniform, indicating that there is a laminar flow region in the furnace zone close to the reaction wall.
- There is a methane concentration gradient above the reaction subtract, with the lowest concentration on the surface.

Subtract location & Deposition rate



The definition method of the position



The deposition rate decreases and then increases along the direction of flow because the velocity boundary layer in the middle of the furnace is thicker.

Conclusions

1. Thermal buoyancy causes temperature and velocity nonuniform near the furnace boundary.
2. Above the subtract, there is a laminar flow region and a methane concentration gradient.
3. The surface deposition rate is related to the thickness of the velocity boundary layer above the substrate, the thicker the boundary layer, the lower the surface deposition rate.