Numerical simulation of evaporation characteristics for heated tobacco products

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Outline

- Background
- Numerical Model
- Numerical Case Setup
- Results and Discussion
- Conclusions

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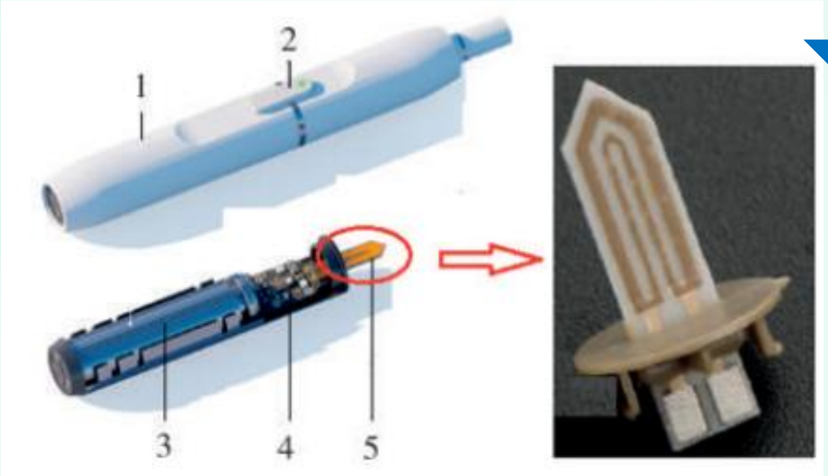
Background



Schematic diagram of sample apparatus and its heating element. [1]

Conventional cigarette: high burning temperature (800℃)

Harmful substrate harmful substances mainly composed of tar

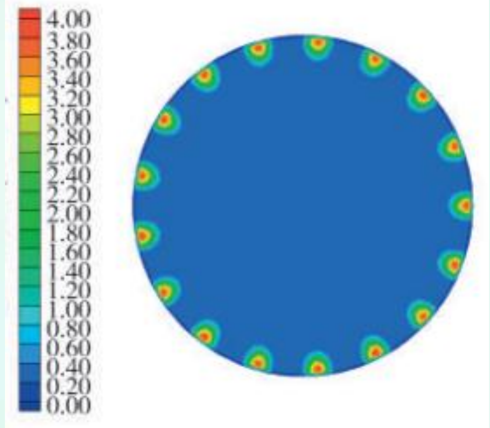
Heated tobacco products: low evaporation temperature (250~350℃)

- The evaporation and capillary transport process of multicomponent mixtures in porous structures involve liquid-vapor interface phase transition mechanisms that are not yet clear.
- The capillary transport mechanisms affected by the gas-liquid-solid triple contact lines in unsaturated porous structures have not been widely accepted.
- The heat and mass transfer phenomena of multi-component mixtures are even more complex.

[1]Chen Chaoying. Change and challenge: outlook for development of new tobacco products[J]. Acta Tabacaria Sinica, 2017, 23(3): 14-18.

Background

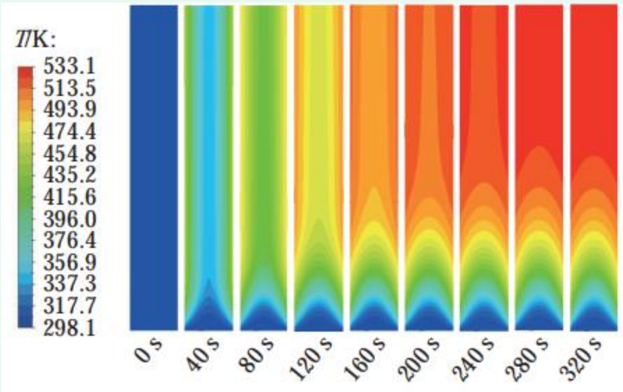
Distribution of smoke velocity at the mouth end of a grooved filter



Sun et al. [1] established a flow and heat transfer model for filters, studied the influence of different groove shapes and sizes on smoke transport and component distribution They found that rectangular groove shapes have a higher proportion of smoke compared to triangular and trapezoidal groove shapes.

[1]Sun Zhiwei, Wen Jianhui, Du Wen, et al. Simulation of flow field distribution of cigarette smoke in grooved filter by computational fluid dynamics[J]. Tobacco Science & Technology, 2018, 51(10): 90-96.

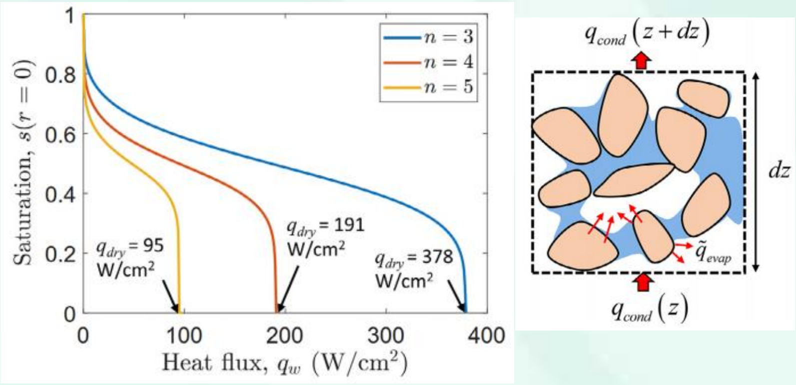
Temperature distribution of cigarette at different time



Xiao et al. [2] established a porous medium flow and heat transfer model and conducted a study on the flow field and temperature field of heated tobacco during the heating and suction process through CFD simulation. They obtained the temperature distribution and heat transfer coefficient of the tobacco segment.

[2]Xiao Weiqiang, Zhou Guojun, Jian Jian, et al. Numerical Simulation of Heat Transfer and Smoke Flow of Heated Cigarette Product[J]. Journal of East China University of Science and Technology, 2021, 47(01): 35-40.

A plot of the liquid saturation of the wick domain as a function of the applied heat flux



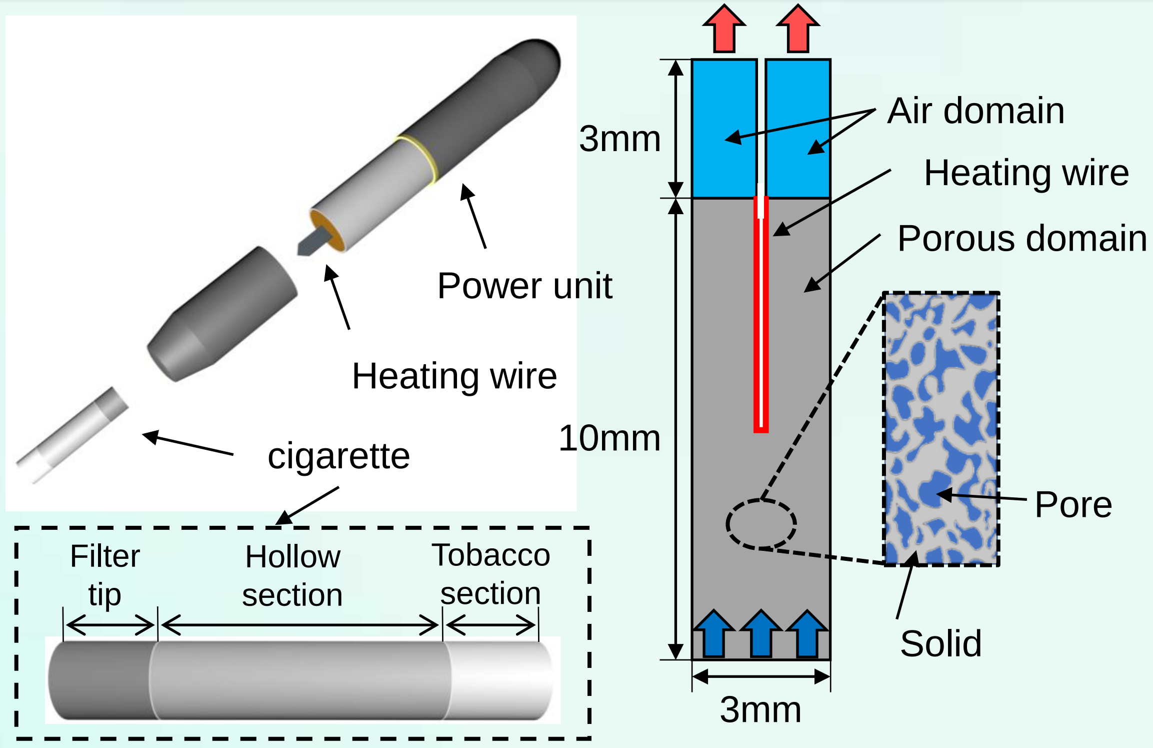
Sudhakar and Garimella [3] established a semi-empirical model for predicting the thermal resistance and critical heat flux during phase change process in porous media, and analyzed the effects of pore size, void fraction, and heater size on the temperature distribution in porous media.

[3] S. Sudhakar et al. A semi-empirical model for thermal resistance and dryout during boiling in thin porous evaporators fed by capillary action[J]. International Journal of Heat and Mass Transfer, 2021, 181: 121887.

Outline

Numerical Model

Schematic diagram of heated tobacco structure and simplified computational domain.



Evaporation process of binary mixed e-liquid within porous cigarette.

Assumption

- The mixture of smoke and air is an incompressible fluid;
- The porous tobacco segment is a uniformly porous medium with a constant porosity;
- The heat transfer model of porous medium adopts the thermal equilibrium equation;
- The thermal physical parameters of e-liquid and porous tobacco segment are constant.

Highlight

Heat transfer model
Species transport model
Capillary model

Eulerian-VOF method
Skjaeveland capillary model

Numerical Model

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Governing equations

Porous evaporation equations

Continuity equation: $$\frac{\partial}{\partial t}(\alpha_q\rho_q) + \nabla\cdot(\alpha_q\rho_q\vec{v}_q) = \sum_{p=1}^{n}(\dot{m}_{pq} - \dot{m}_{qp}) + S_q$$

The momentum equation includes an additional momentum source term.

$$\frac{\partial(\gamma\alpha_q\rho_q\phi_q)}{\partial t} + \nabla\cdot(\gamma\alpha_q\rho_q\vec{v}_q\phi_q) = \nabla\cdot(\gamma\Gamma_q\nabla\phi_q) + \gamma S_{\phi,q}$$

By replacing the actual pore structure with empirically-based flow resistance, the momentum source term includes viscous loss and inertial loss terms.

$$S_i = -\left(\frac{\mu}{\alpha}v_i + C_2\frac{1}{2}\rho|v|v_i\right) \qquad C_1 = \frac{1}{\alpha}$$

The energy equation for the porous medium adopts the thermal equilibrium equation.

$$\frac{\partial}{\partial t}(\gamma\rho_f E_f + (1-\gamma)\rho_s E_s) + \nabla\cdot\left(\vec{v}(\rho_f E_f + p)\right) = S_f^h + \nabla\cdot\left[k_{eff}\nabla T - \left(\sum_i h_i J_i\right) + (\bar{\tau}\cdot\vec{v})\right]$$

Capillary force equations

The capillary pressure under a curved phase interface can be calculated by the Young-Laplace equation.

$$P_c = P_{nw} - P_w = \sigma\left(\frac{1}{R_1} + \frac{1}{R_2}\right)$$

the Skjaeveland model is selected to simulate the capillary pressure variation of phase interfaces inside the porous medium. [1]

$$P_{c,q} = \frac{P_{e,w}}{\left(\frac{(\alpha_q - \alpha_{qr})}{(1-\alpha_{qr})}\right)^{a_w}} - \frac{P_{e,nw}}{\left(\frac{(1-\alpha_q-\alpha_{pr})}{(1-\alpha_{pr})}\right)^{a_{nw}}}$$

Inlet pressure (P_e) is the minimum pressure required for the liquid to pass through the maximum pore size in the porous medium. $\lambda=1/a$ represents the pore size distribution index.

[1]M. Th. Van. Genuchten. A Closed-form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils [J]. Soil Science Society of America Journal, 1980, 44(5): 892-898.

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Numerical Case Setup

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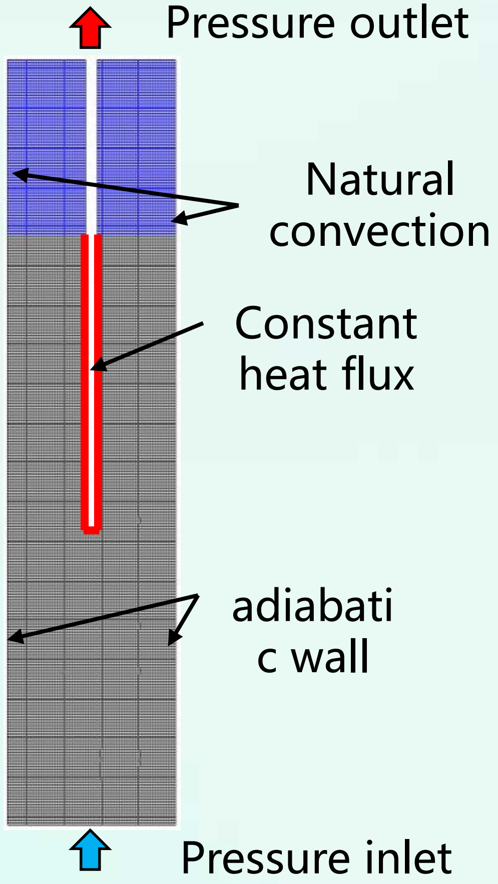
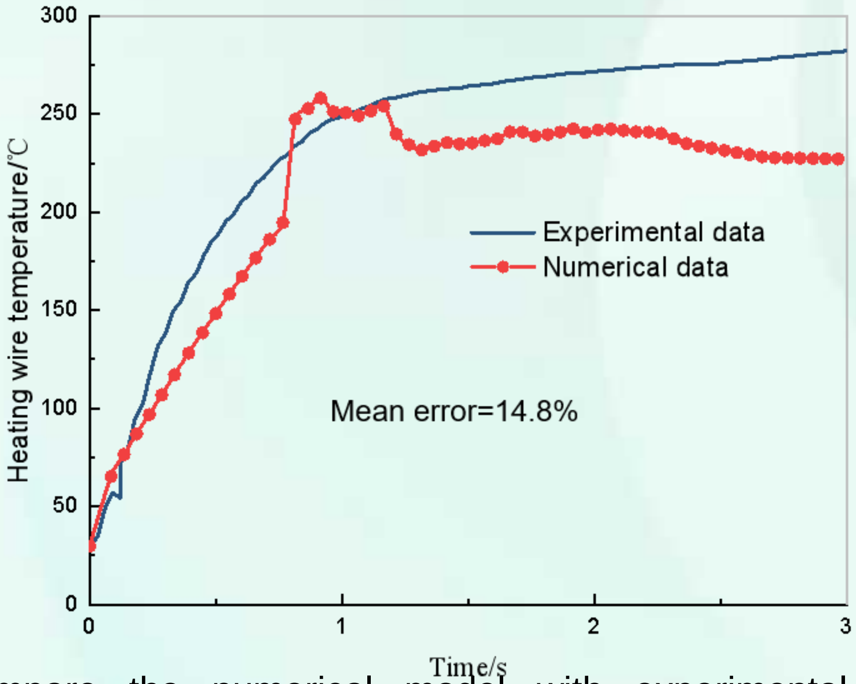
Boundary conditions



Model validation



Compare the numerical model with experimental data in reference [1].

Under the condition of selecting the experimental e-liquid component in the literature as propylene glycol: glycerin = 1:1 and heating power of 9.09 W, heat the model for 3 seconds. The average relative error is 14.8%.

[1]Li Dian, Gao Yihan, Li Zhihua, et al. Similarity experiment on temperature characteristics of e-cigarette and establishment of scaledmodel experimental platform[J]. Acta Tabacaria Sinica, 2020, 26(05): 10-17.

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Results and Discussion

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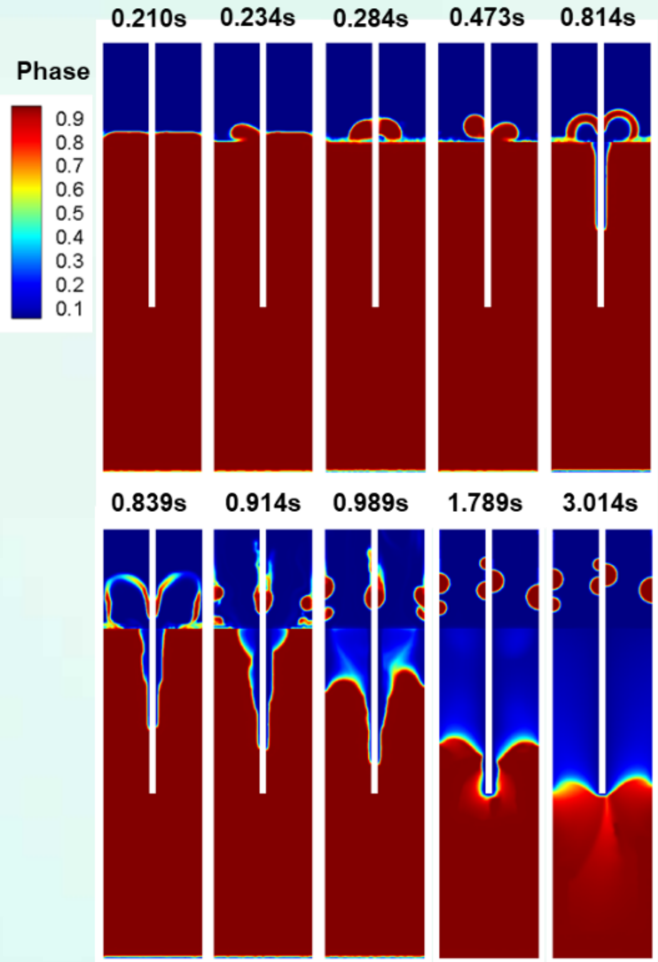
Phase distribution



Phase distribution with a porosity of 0.4 and heating power of 6 W

t = 0.234~0.473 s

The liquid film retracts and forms a spherical shape, and the liquid bridge breaks, causing the liquid droplet to slightly bounce up.

t = 0.473~0.814 s

Boiling occurs inside the porous medium. The rapidly generated vapor pushes the surface droplets, forming a circular ring.

t = 0.814~0.914 s

The liquid ring breaks and forms many small droplets attached to the sidewall surface.

t = 0.989~3.014 s

The liquid-vapor interface in the porous domain gradually decreases with the progress of evaporation.

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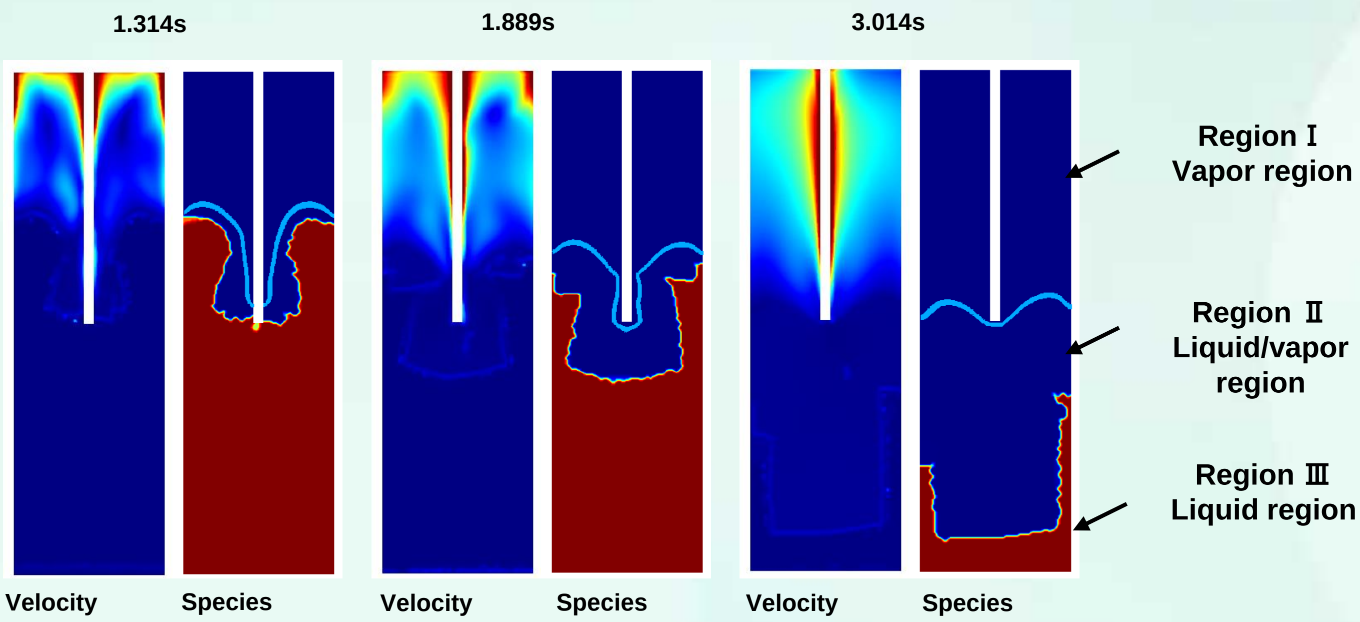
Velocity distribution



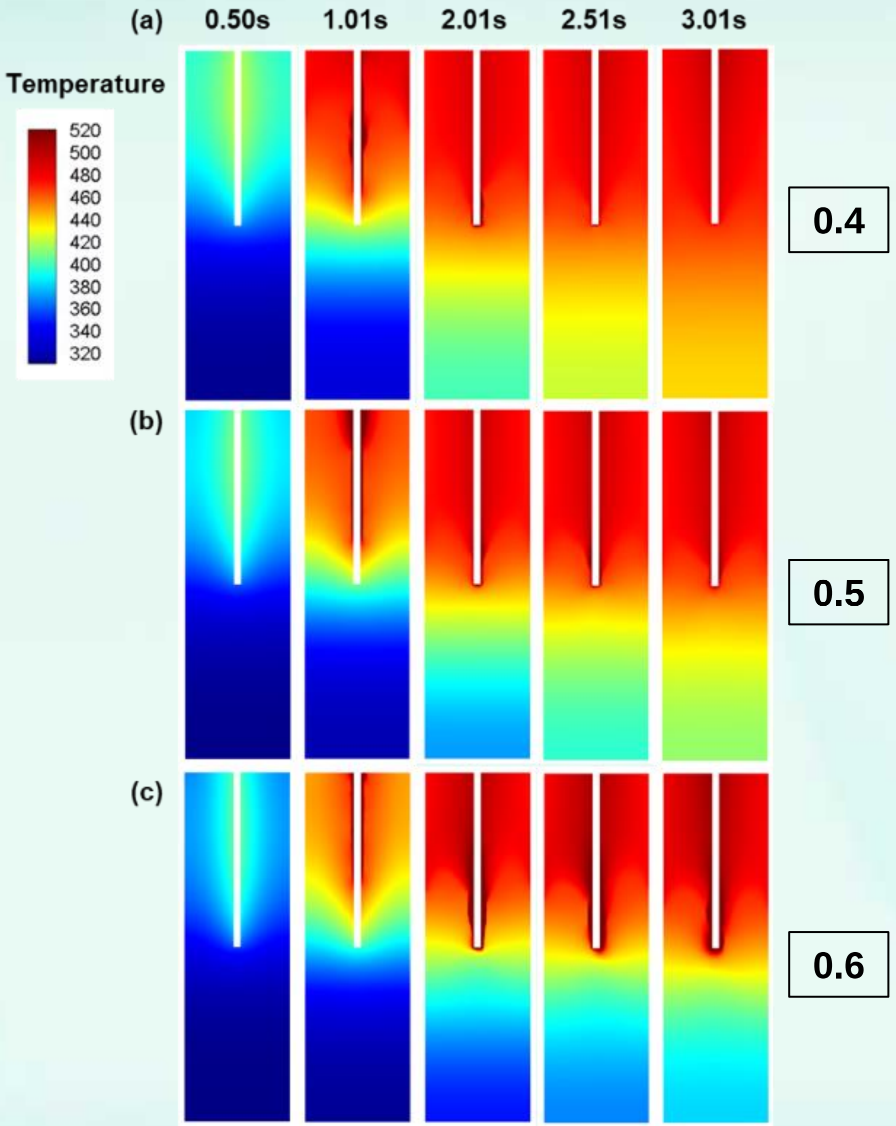
Region Ⅰ: The fluid velocity is high because the region is full of vapor. And the low viscosity of vapor makes it easier to flow in the porous domain.

Region Ⅱ: The evaporation on the surface of the liquid-vapor interface promotes the migration of vapor phase and liquid phase, increasing the flow rate at the boundary.

Region Ⅲ: The fluid velocity is low due to the high viscosity of liquid in porous domain.

Results and Discussion

Porosity effect



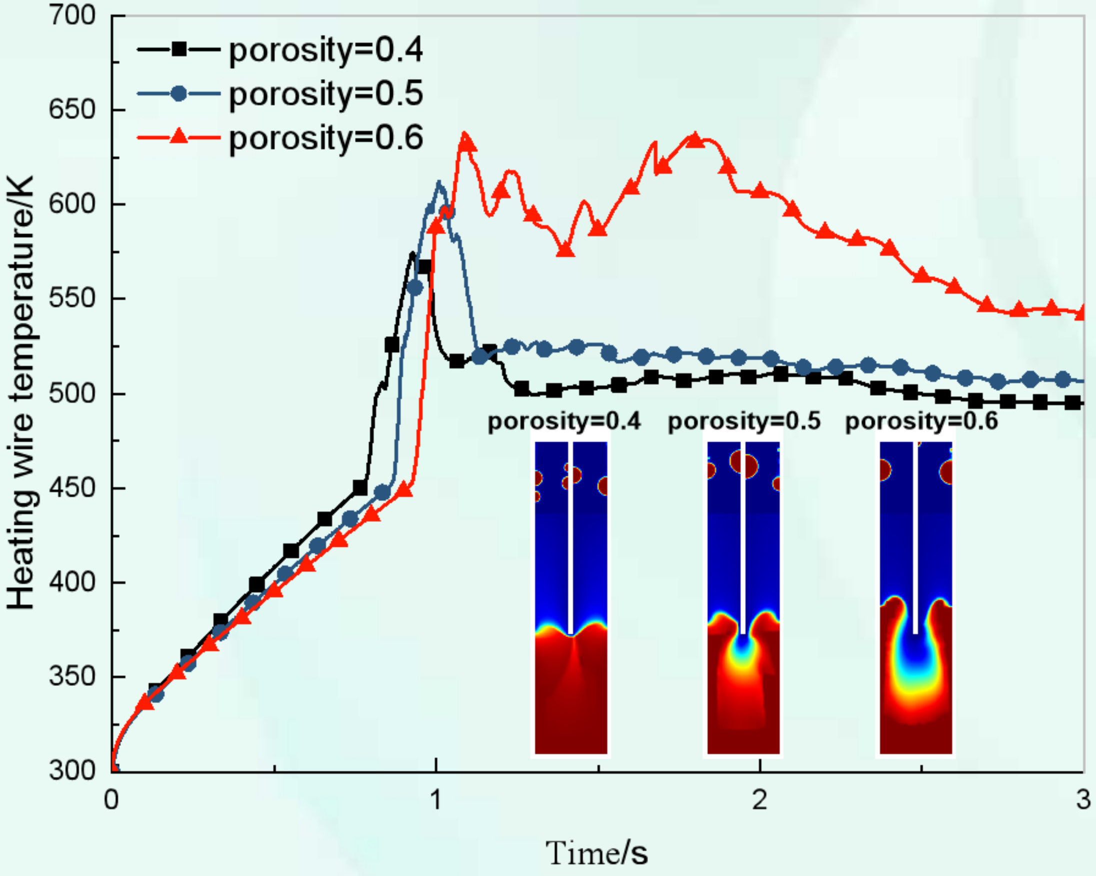
Temperature distribution for different porosities, (a) 0.4, (b) 0.5, and (c) 0.6, in the porous domain.

- As the porosity increases, the highest temperature and the temperature after stabilization of the porous domain also increase.
- After the liquid film disappears, the influence of effective thermal conductivity becomes dominant. Moreover, the viscous force coefficient and the inertia force coefficient decrease, causing the velocity of vapor accelerates, promotes vapor overflow from the porous domain, which further strengthens evaporation.

Results and Discussion

Porosity effect

- Initially, the temperature within the porous medium did not reach the saturation temperature of the liquid, and the temperature variation with time was basically linear.
- Subsequently, a violent evaporation process occurred within the porous medium, and the slope of the temperature curve rapidly increased due to the generation of vapor. The effective thermal conductivity of the porous medium was reduced because of the partly filled porous medium, resulting in heat accumulation.
- When the temperature rose to a certain point, the heating surface began to cool down because after the liquid film ruptured, the flow rate of vapor increased, carrying away some heat.
- Finally, when the supplied heat and heat dissipation of steam reached equilibrium, the temperature gradually stabilized.



Variation of heating wire temperature over time for different porosities.

Results and Discussion

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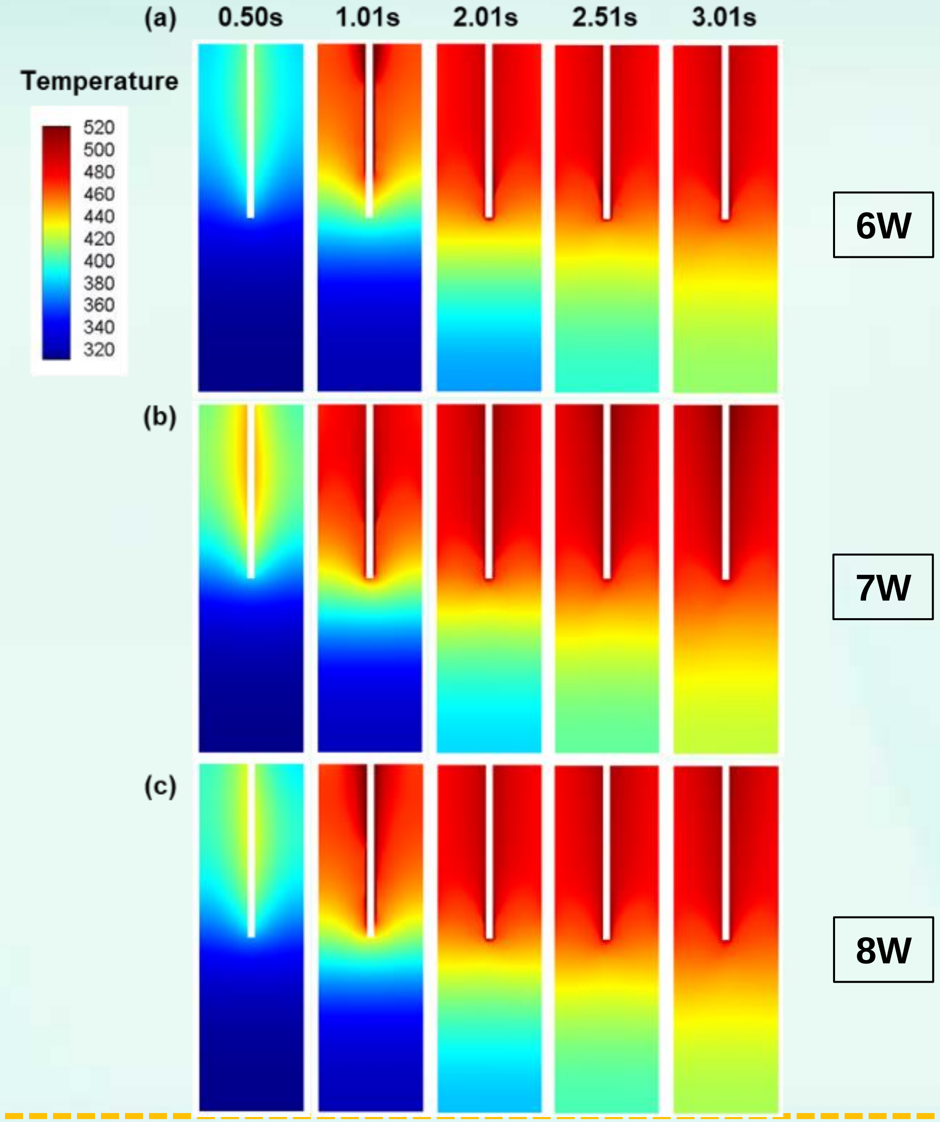
Power effect



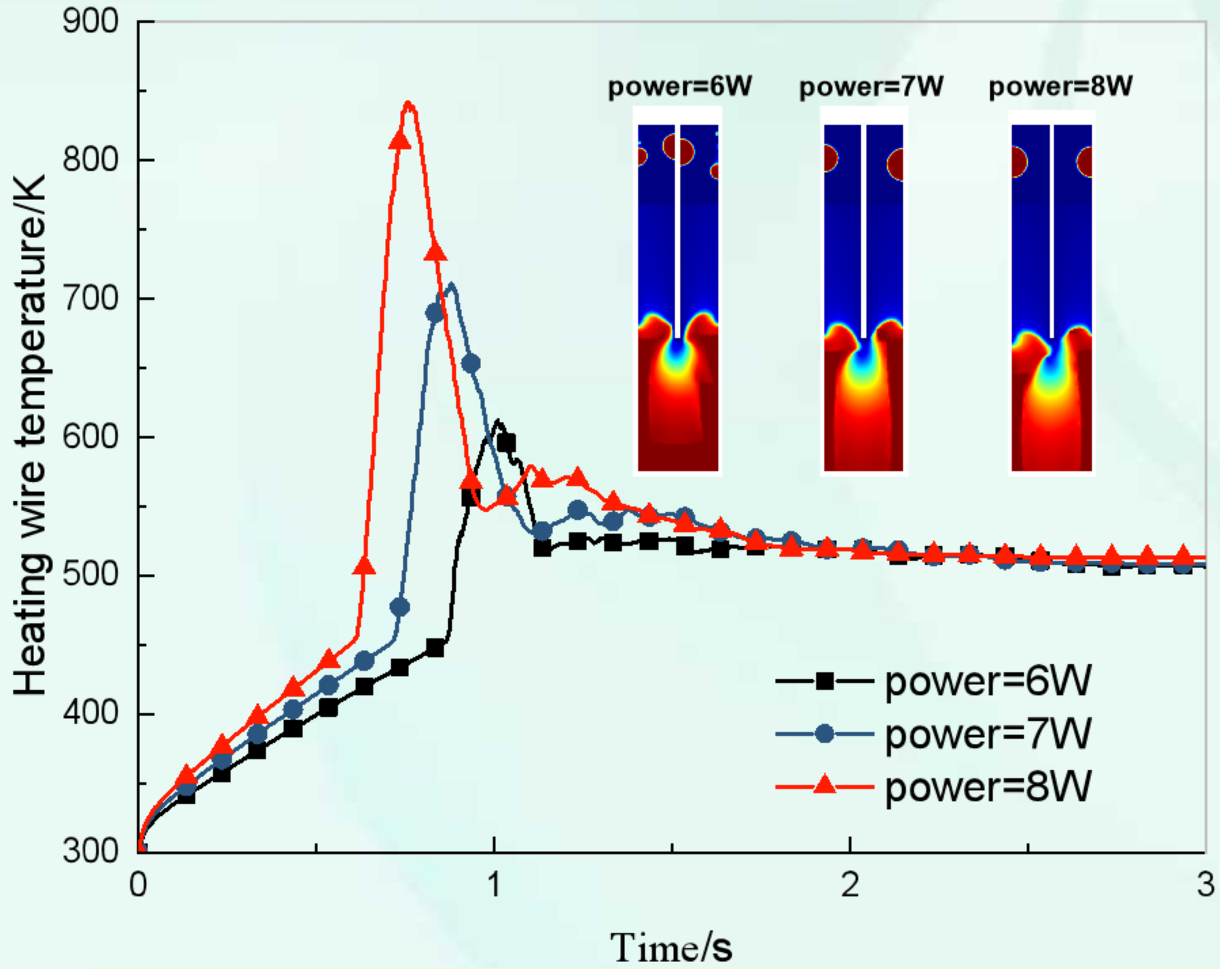
- With the increase in power, the temperature remains consistent after stabilization. This indicates that the effective thermal conductivity, inertial force coefficient, and viscosity coefficient of the porous medium have a significant impact on evaporation, resulting in the gas-liquid interface remaining almost consistent after stabilization.

Temperature distribution for different heating power, (a) 6 W, (b) 7 W, and (c) 8 W, in the porous domain.

Results and Discussion

Power effect

- In the single-phase region, the heating surface temperature rises quickly and the highest temperature also increases as the heat increases, influenced by the liquid film coverage. However, after stabilization, the temperature differences are relatively small at three different heating powers, with a temperature difference of less than 8K.
- In the early stage of evaporation, the temperature increase is more obvious with the increase in power due to the close contact between the liquid-vapor interface and heating surface.
- In the later stage, when the liquid-vapor interface is far away from the heating surface, the parameters of the porous structure play a dominant role in the evaporation process, and the remaining heat is dissipated by the heating surface to the air domain, maintaining the temperature of the heating surface.



Variation of heating wire temperature over time for different heating power.

Outline

Conclusions

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- In the single-phase region, the temperature of the heating surface increases linearly. After exceeding the boiling starting point, the slope of the temperature curve rises rapidly. When it reaches the highest point, the temperature begins to decrease due to the influence of liquid film rupture, and finally reaches a steady state.

- Due to the combined effect of liquid film dynamics behavior and porous structure parameters (effective thermal conductivity, inertia force coefficient and viscous force coefficient). As the porosity increases, the temperature rise rate of the porous domain slows down in the single-phase region, the boiling starting point is postponed, and the highest temperature and the temperature after stabilization are both increased.

Conclusions

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- With the increase of heating power, the temperature rise rate of the porous domain in the single-phase region accelerates, and the maximum temperature also increases significantly.

- The heating power plays a dominant role in the early stage of evaporation, while the effect of porous structure parameters is greater in the later stage of evaporation. Although the heating power is inconsistent, with the same porous structure, the final stable vapor-liquid interface and the temperature of the heating surface are basically the same.

Thanks for your listening !

Q&A

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