Modeling the Melting Process of Quartz Glass using SPH Method

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Outline

- Background
- Geometry Models
- Mathematical Models
- Results & Discussions
- Conclusions

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Background

King of Glass

All images come from internet.

Quartz glass has become an indispensable material in modern science technology and industry due to good thermo-physical property, excellent optical performance and outstanding electrical property.

Background

A new two-step technology

Deposited by flame fused technique

Removed hydroxyl in electrical melting vacuum furnace

A new two-step process has been developed by modifying the technique in existence.

Traditional numerical methods based on grid

	Lagrangian grid	Eulerian grid
Grid	Fixed on the material	Fixed on the space
Boundary	Track and determine simply	Track and determine difficulty
Complicated geometries	Conveniently	Inconveniently
Large deformation	Difficulty	Simple

Meshfree methods

Melting process

large deformation

free surface

heat transfer

SPH：effective tool

Background

Our interests

The quality of quartz glass, such as bubble rate, hydroxyl content, homogeneity, is mainly controlled by the temperature and flow filed during melting process. The main interest is placed on **the research of melting process** that remove hydroxyl and bubble.

Our challenges

- Physical viscosity in flow flied:
  - Monaghan type artificial viscosity
  - Morris physical viscosity model
- Thermal radiation transfer in SPH framework:
  - Radiative heat transfer on surface: adding a heat source to replace the thermal energy;
  - Radiative heat transfer in participating media: an effective thermal conductivity based on **Rosseland model**

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Physical Models

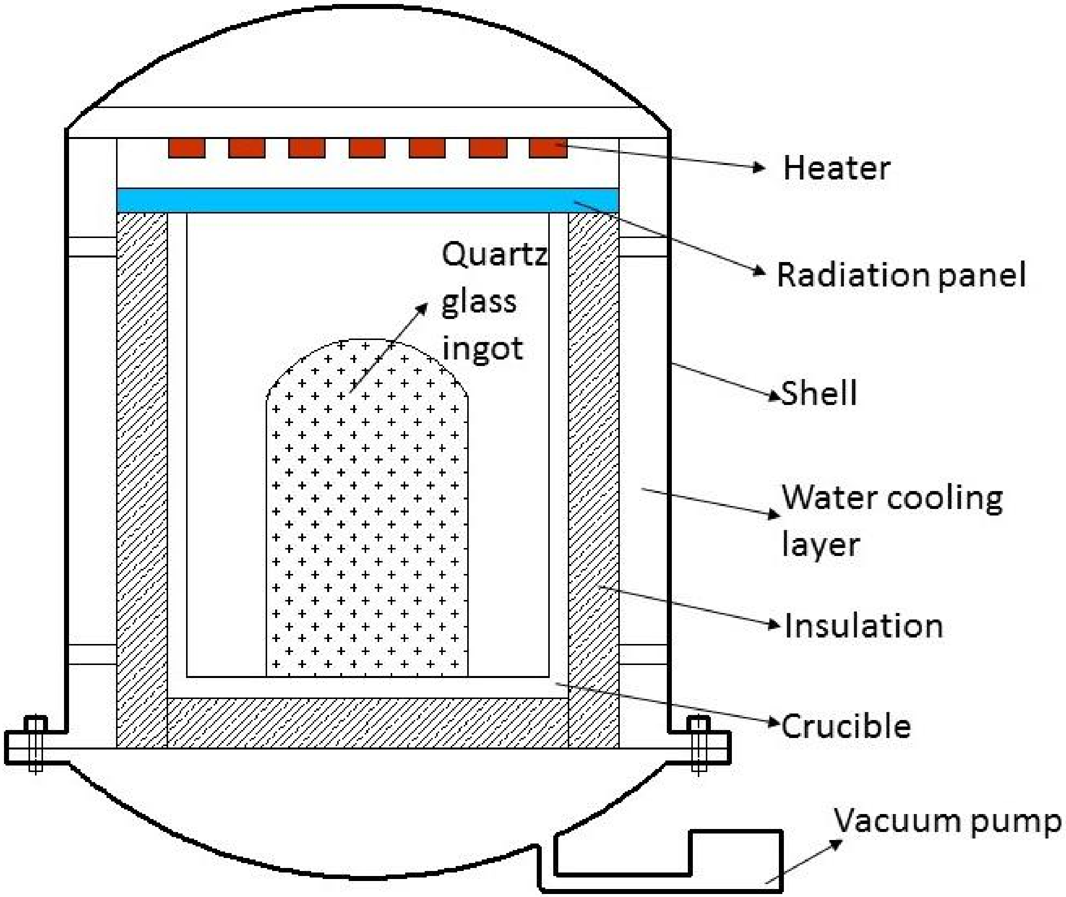

Fig. 1 Sketch of the quartz ingot in an electric melting furnace.

Physical Models

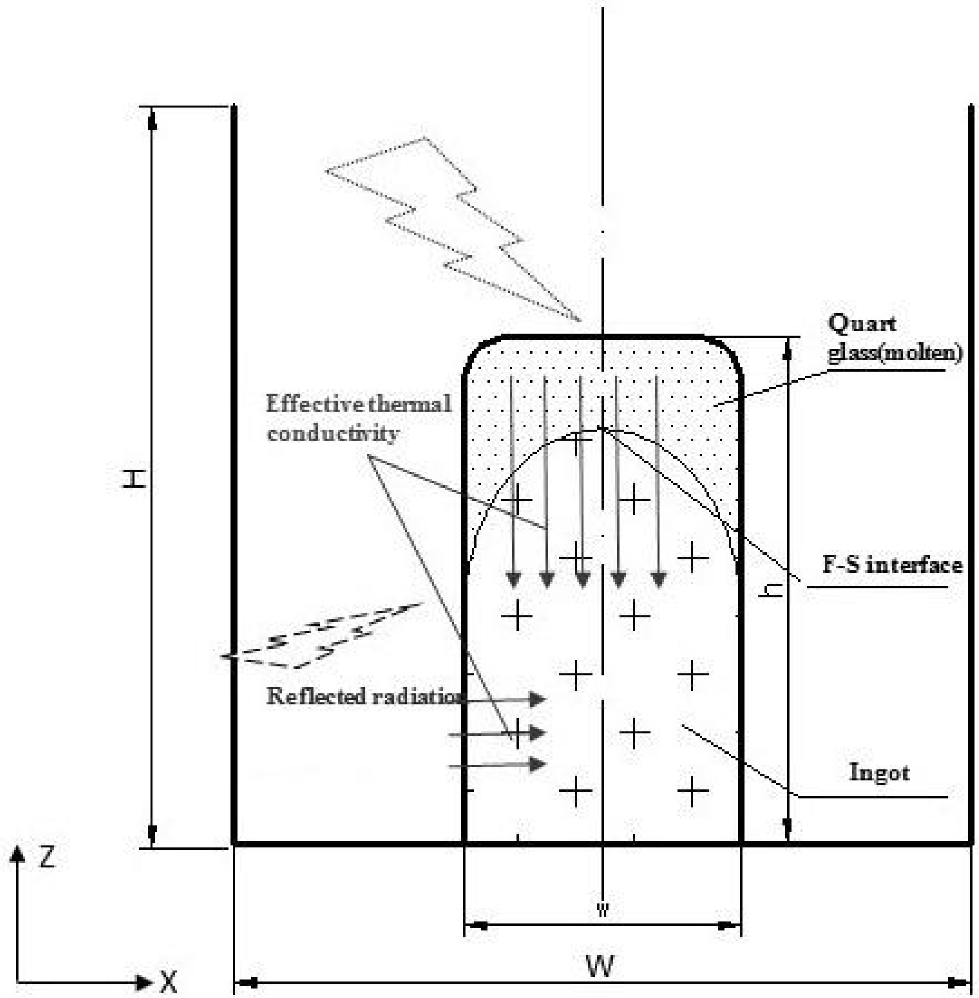

Fig.2 Description of heat transfer during the ingot melting.

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- **Mathematical Models**
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Mathematical models

➢ Computational Fluid Dynamics (CFD) theory

Mass Conservation: $$\frac{D\rho}{Dt} = -\rho\nabla\cdot v$$

Momentum Conservation: $$\frac{Dv}{Dt} = -\frac{1}{\rho}\nabla p + \frac{1}{\rho}\boxed{\nabla\cdot\tau} + g$$

Energy Conservation: $$\frac{De}{Dt} = \frac{p}{\rho}\nabla\cdot v + \nabla\cdot(\kappa_{eff}\nabla T)$$

where $$\kappa_{eff} = \kappa + \kappa_r$$

Second Derivative

$$\Pi_{ij} = \begin{cases} \dfrac{-\alpha_1 \overline{c_{ij}}\phi_{ij} + \beta_1\phi_{ij}^2}{\overline{\rho_{ij}}}, & v_{ij}\cdot r_{ij} < 0 \\ 0, & v_{ij}\cdot r_{ij} \geq 0 \end{cases}$$

or

$$\mu\nabla^2 V$$

Mathematical models

➢ Numerical scheme of SPH form

Basic theory of SPH

Kernel approximation: $$< f(r) >= \int_{\Omega} f(r')W(r-r',h)dr'$$

Particle approximation: $$< f(r_i) >= \sum_{j=1}^{N} \frac{m_j}{\rho_j} f(r_j) \cdot W(r_i - r_j, h)$$

Spatial derivative:

$$\nabla \cdot f(r_i) = \frac{1}{\rho_i}[\sum_{j=1}^{N} m_j[f(r_j) - f(r_i)] \cdot \nabla_i W(r_i - r_j, h)]$$

or

$$\nabla \cdot f(r_i) = \rho_i[\sum_{j=1}^{N} m_j [\left(\frac{f(x_j)}{\rho_j^2} + \frac{f(x_i)}{\rho_i^2}\right] \cdot \nabla_i W\left(r_i - r_j, h\right)]$$

Mathematical models

spheric
ERCOFTAC

CFD governing equations in SPH

$$\frac{D\rho_i}{Dt} = \rho_i \sum_{j=1}^{N} \frac{m_j}{\rho_j} v_{ij} \cdot \nabla_{ij} W$$

$$\frac{D v_i^\alpha}{Dt} = \sum_{j=1}^{N} m_j \left(\frac{p_j}{\rho_i^2} + \frac{p_i}{\rho_i^2}\right) \frac{\partial W_{ij}}{\partial x_i^\alpha} + F$$

$$\frac{De_i}{Dt} = \frac{1}{2} \sum_{j=1}^{N} m_j \left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2}\right) v_{ij} \nabla_{ij} W + \nabla \cdot (\kappa_{eff} \nabla T)_i$$

Second derivative in SPH form

The method of finite difference combined with the first derivative in SPH form

$$\nabla \bullet (\kappa_{eff} \nabla \mathrm{T})_i = \sum_{j=1}^{N} \frac{4m_j}{\rho_j \rho_i} \frac{\kappa_i \kappa_j}{(\kappa_i + \kappa_j)} (T_i - T_j) \frac{r_{ij} \bullet \nabla_{ij} W}{r_{ij}^2 + \zeta^2}$$

$$\geqq \bullet \tau_i = (\mu \nabla^2 v)_i^\alpha = \sum_{j=1}^{N} m_j \frac{\mu_i + \mu_j}{\rho_i + \rho_j} v_{ij}^\alpha \frac{r_{ij} \bullet \nabla_{ij} W}{r_{ij}^2 + \zeta^2}$$

Mathematical models

➢ Radiation model & Surface detection

Surface-to-Surface Radiation

A heat source is added to the particles which locate at the surface. And the detailed temperature distribution comes from the CFD results.

Radiation in Participating Media

Rosseland approximation:

$$q_r = -\frac{4\sigma}{3\beta_r}\nabla(n^2T^4)$$

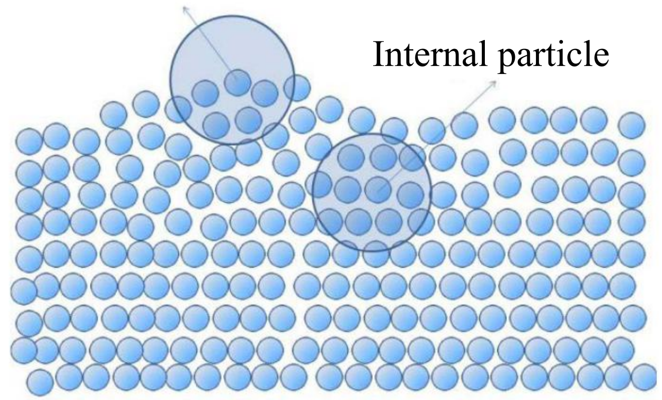
When the refractive index is a constant:

$$q_r = -\kappa_r \Delta T \quad \text{with} \quad \kappa_r = \frac{16n^2\sigma T^3}{3\beta_r}$$

Particle Number Density

$$N_i = \sum_j \left(\frac{m_j}{\rho_j}\right) W(r_i - r_j, h)$$

Lower particle number density on the surface



The particles located at free surface have a lower particle number density than that the inner.[1]

[1] Nbsp, Suprijadi, Faizal F, et al. Journal of Modern Physics, 2014, 05(3): 112-116.

Mathematical models

➢ Numerical Calculation Configuration

- All simulations are performed by modified SPHysics code.
- Equation of state: $p = B\left(\left(\frac{\rho}{\rho_o}\right)^{\gamma} - 1\right)$,where γ=7.

- Two-dimensional areal model: *0.5m*0.5m*,
  The glass ingot dimensions: *0.3m*0.4m*.
- Particles number:
  Fluid particles: *3240*, Boundary particles: *303*
- Initial temperature: *1650K*
- Specific heat capacity: *1500J/(K*kg)*
- Equivalent thermal conductivity: *500 W/(m*K)*
- Density: *1000kg/m³*

Keep same during simulating

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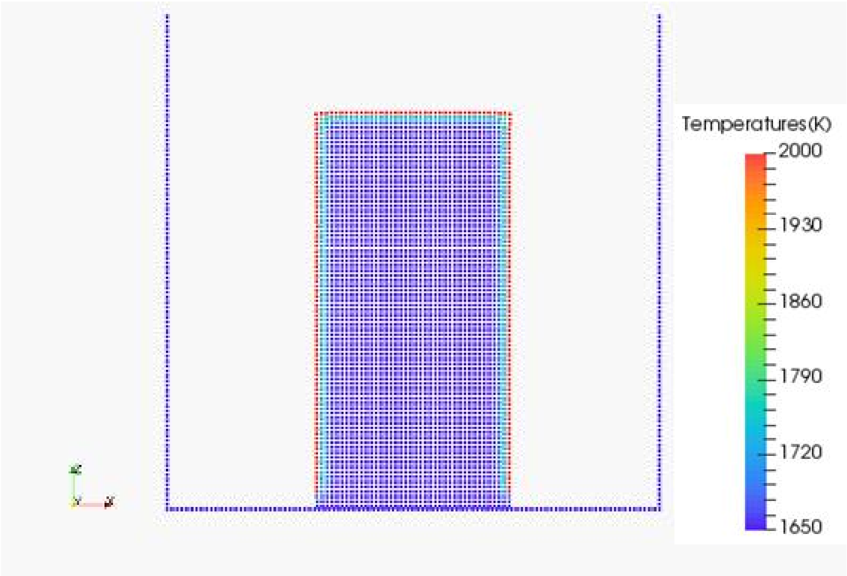
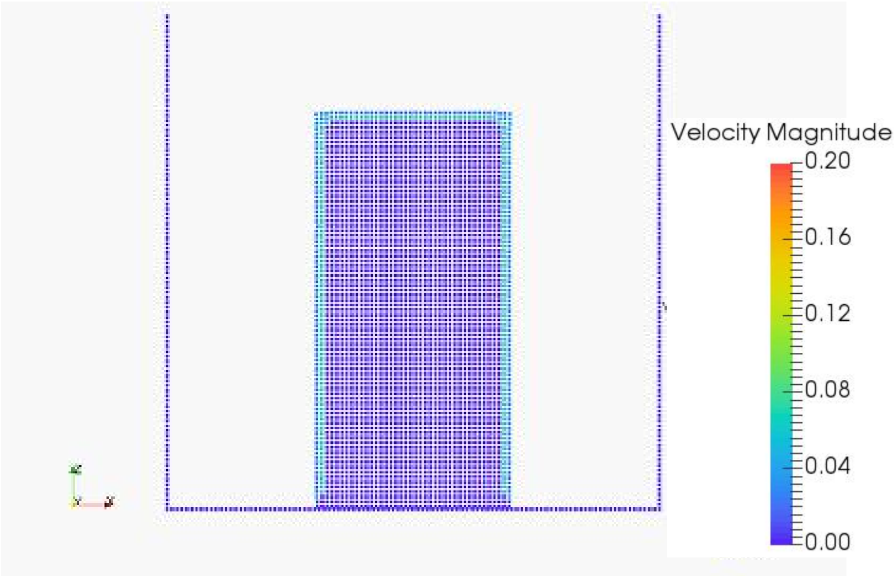
Results & Discussions

➢ Overview of temperature and velocity field



(a) Temperature field



(b)Velocity magnitude field

Fig.3 Velocity field and temperature field distribution of quartz glass melting process(Monaghan artificial viscosity).

Results & Discussions

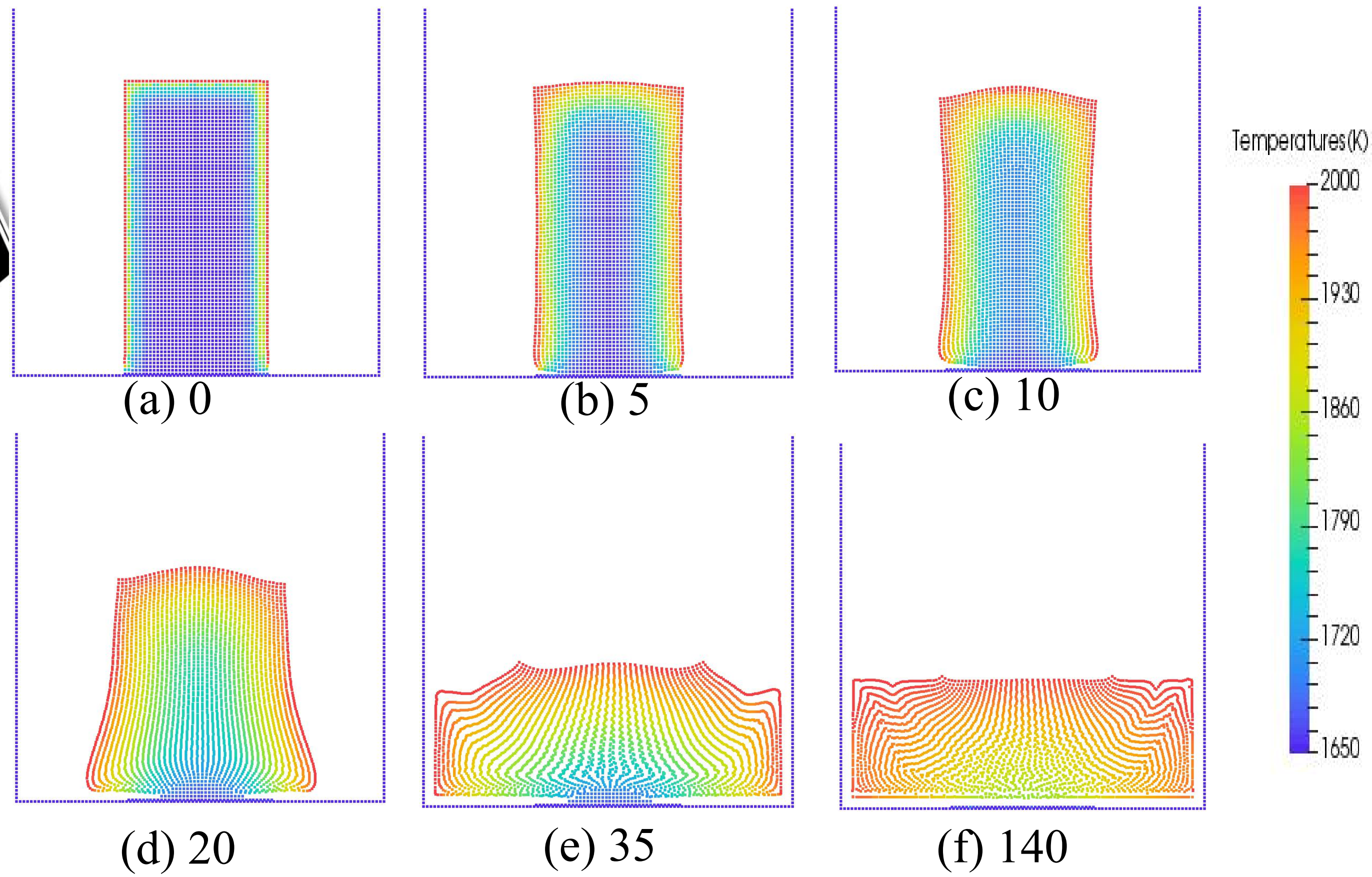


Fig.4 Temperature field distribution of quartz glass melting process (artificial viscosity model).

Results & Discussions

➢ Detection coefficient effect

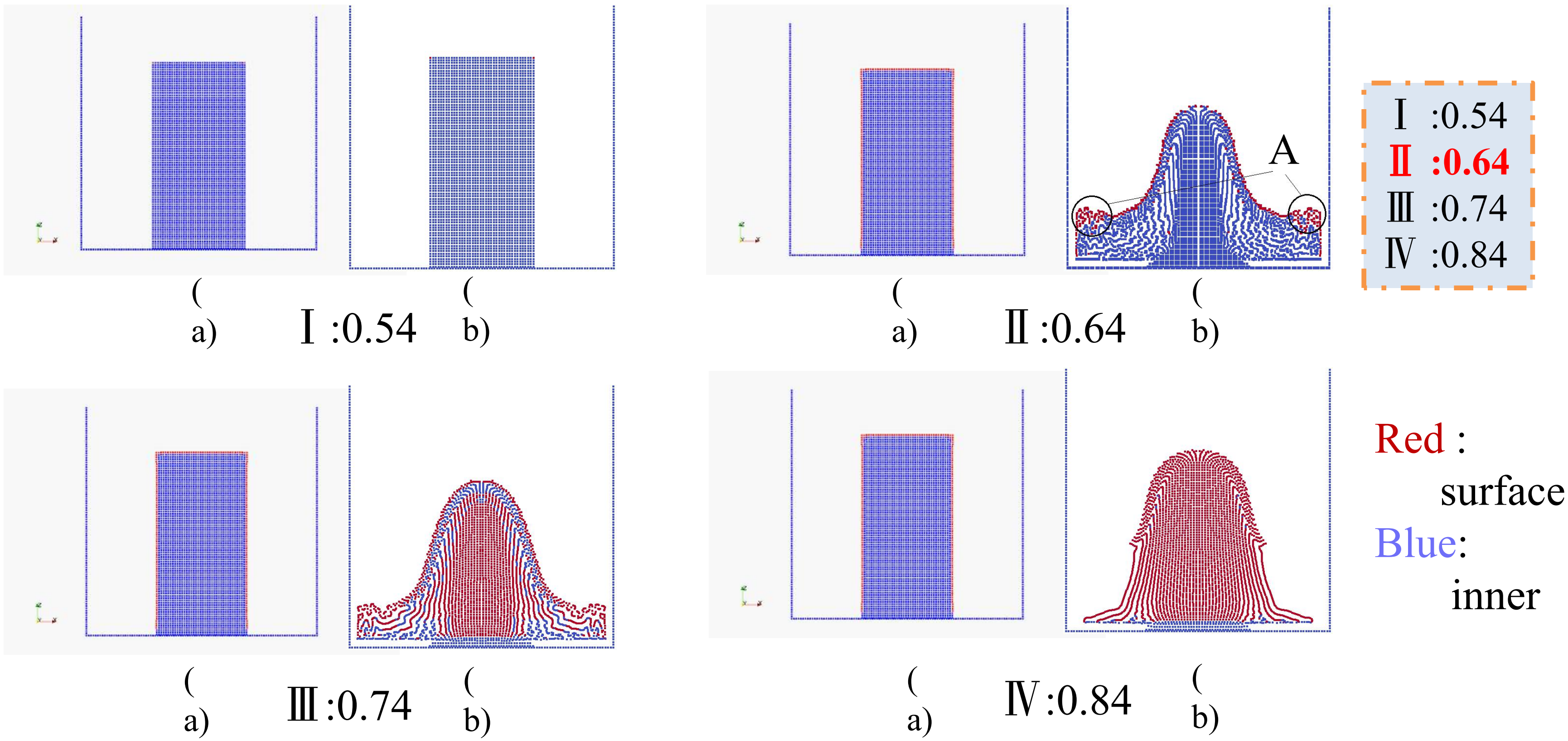
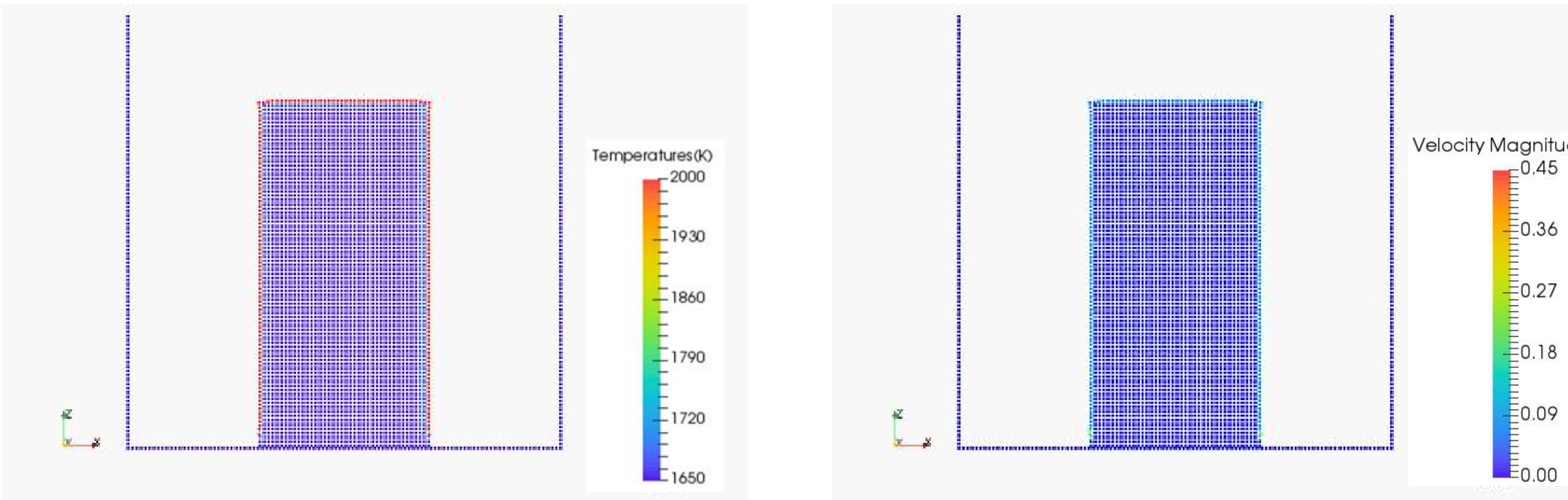


Fig.5 The results of the free surface determination under different detection coefficients. (a) Animation of process; and (b) Results at the time step with maximum error.

Results & Discussions

➢ Dynamic viscosity effect



(a) (b)

Fig.6 The dynamical overview of melting process with the viscosity equaling to 10.

The above shows the quartz glass melting process using the Physical Viscosity model [2] with a similar setting as the artificial viscosity model, and its dynamic viscosity μ equals to 10 $Pa{\cdot}s$.

[2] Morris J P, Fox P J, Zhu Y, et al. Journal of Computational Physics, 1997, 136(1): 214-226.

Results & Discussions

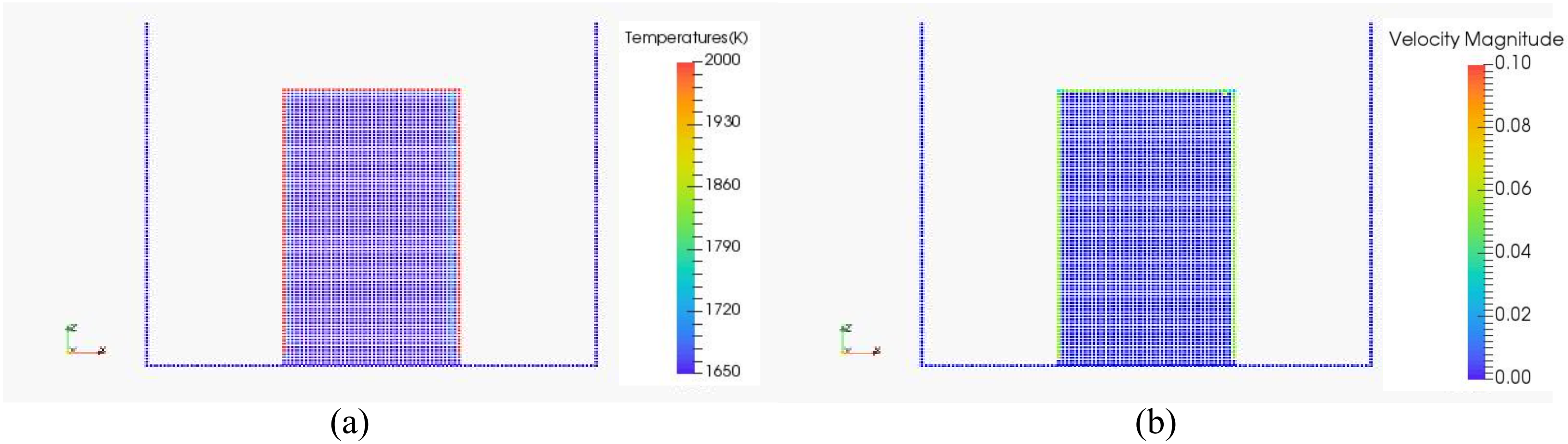


Fig.7 The dynamical overview of melting process with the viscosity equaling to 300.

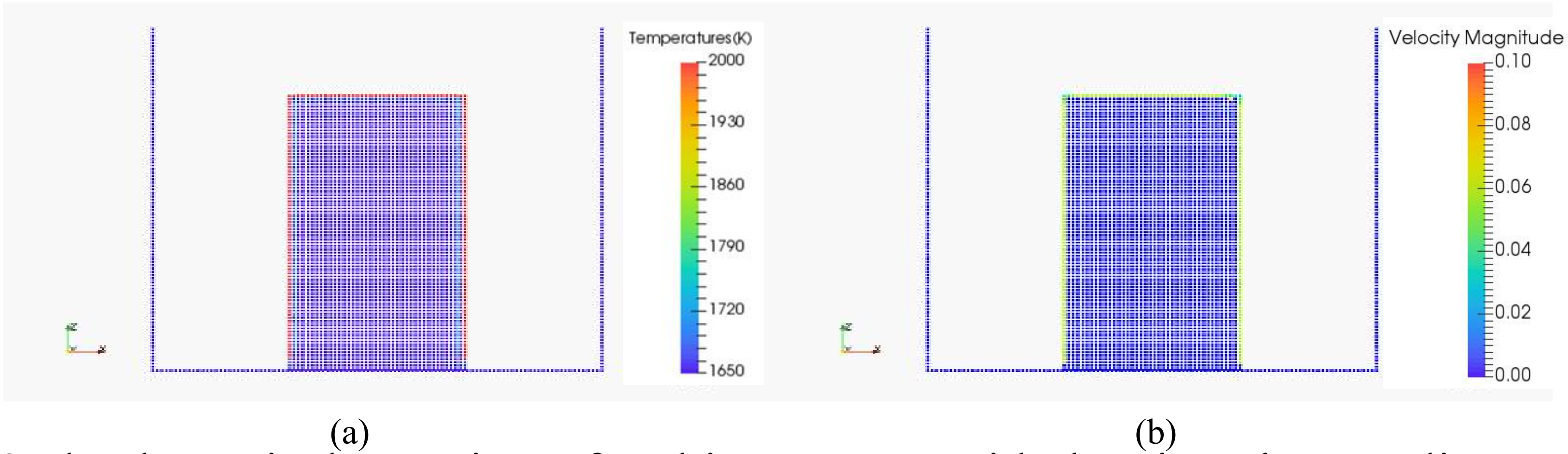


Fig.8 The dynamical overview of melting process with the viscosity equaling to 500.

Results & Discussions

➢ Incomplete melting phenomenon

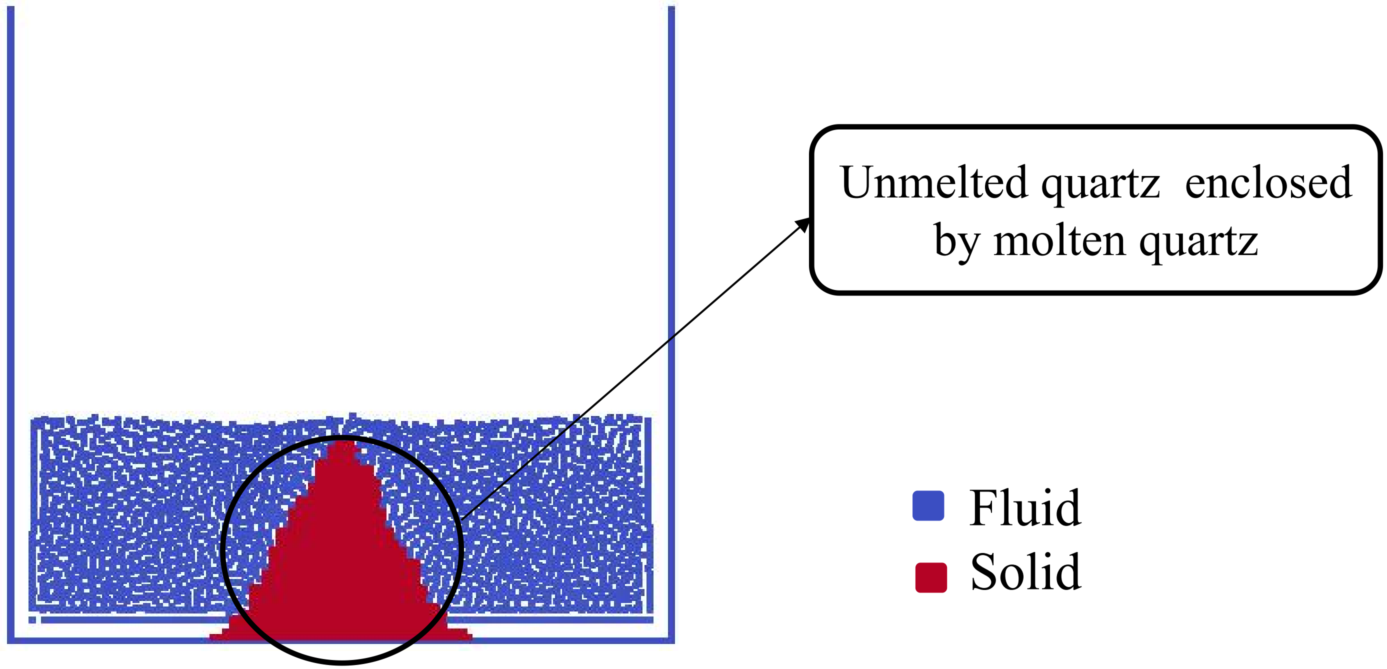


Fig. 9 Morphology with dynamic viscosity equaling to 10 at the end of the melting process.

- The unmelted quartz suffers from a terrible heating condition.
- The unmelted quartz may cause critical defects degrading optical uniformity.

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Conclusions

The SPH algorithm based on SPHysics coupled heat transfer and high-viscosity flow is employed. Based on analysis of melting process, the following conclusions can be drawn:

- Artificial viscosity model and physical viscosity model proposed by Morris take good account of the dissipation phenomenon in highly viscous fluid flow. However, physical viscosity model is more practical in physical significance.
- The algorithm based on the particle density is applied to track the free surface, and a suitable detection coefficient is found to be *0.64* in the current study.
- By analysing the cases, the morphology of the melting process is dependent on the combined effect of the liquid viscosity and the heat transfer rate.
- According to the modelling results, there would be solid quartz in the centre of the crucible that cannot be melted due to weak heat transfer to the centre.

Acknowledgements

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Thanks for listening!