Mathematical Modelling and Numerical Investigation of Industry and Environment Related Processes – A Multiscale Approach

Presented by

Abhiram Hens, PhD

Assistant Professor, Department of Chemical Engineering
Associate Dean (Research & Consultancy)

National Institute of Technology Durgapur
M.G. Avenue, Durgapur - 713209

Background

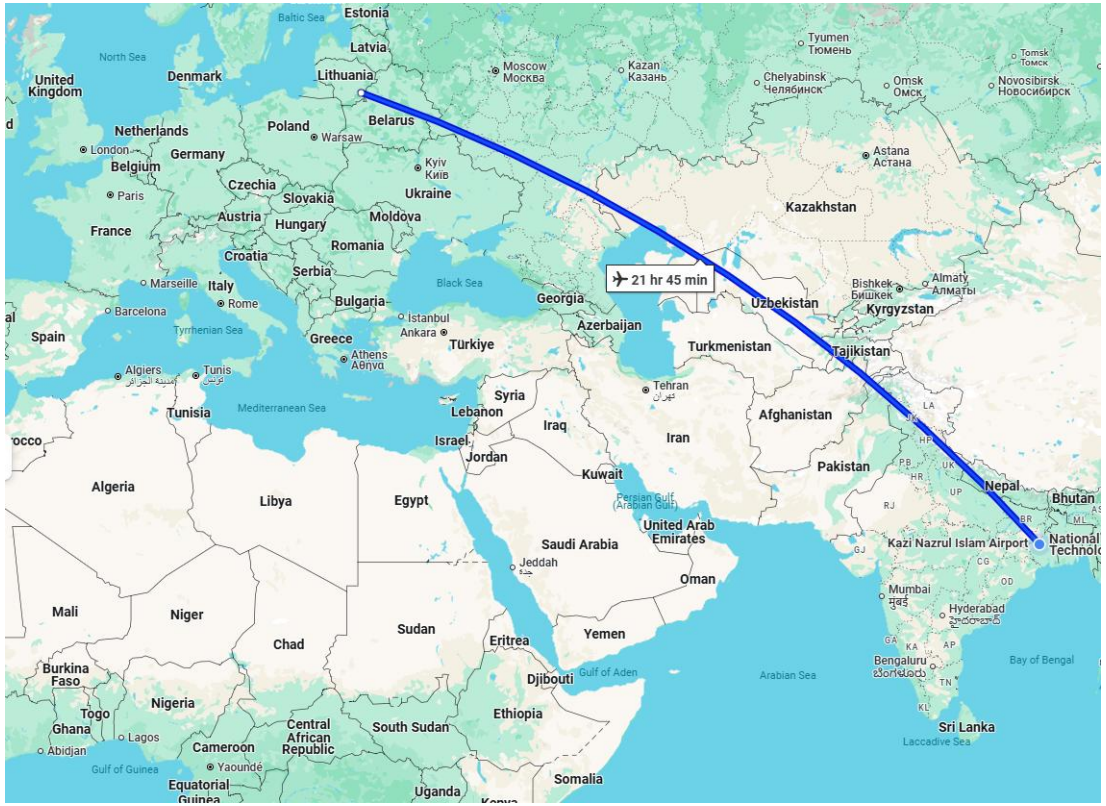
MoU between NIT Durgapur and Vilnius Tech, Lithuania

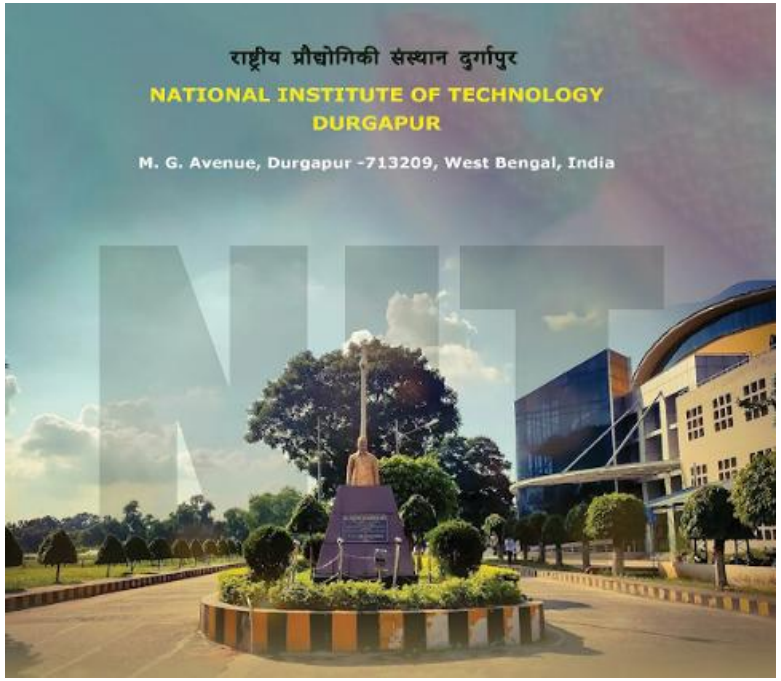
Faculty Exchange

Collaborative Research Visit and Research Interaction

Host:

Prof. Dr Edita BALTRĖNAITĖ-GEDIENĖ
Institute of Environmental Protection
Department of Environmental Protection and Water Engineering
Vilnius Gediminas Technical University



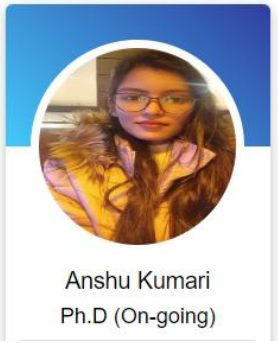


My Research Area

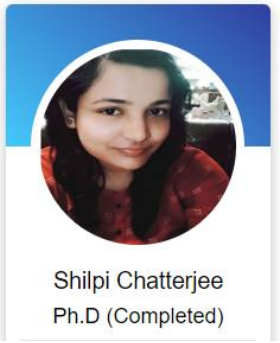
- **Computational Fluid Dynamics and Heat Transfer**
- **Molecular Dynamics Simulations**
- **Droplet and bubble dynamics**
- **Development of Software for Chemical Process and Process Safety Analysis**
- **Microfluidics and Nanotechnology**

Collaborations with experimentalists and industry

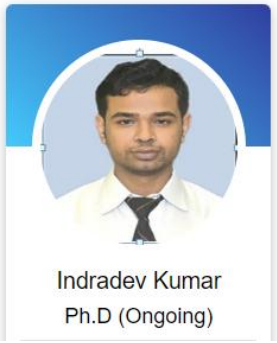
My Research Group



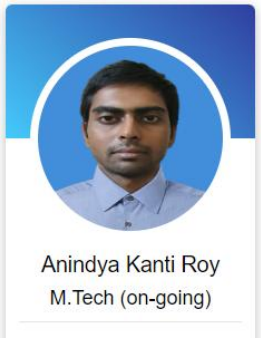
Anshu Kumari
Ph.D (On-going)



Shilpi Chatterjee
Ph.D (Completed)

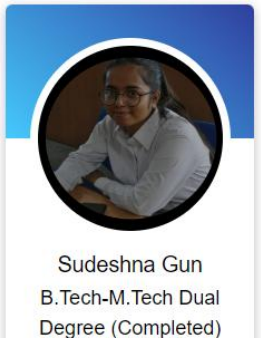


Indradev Kumar
Ph.D (Ongoing)



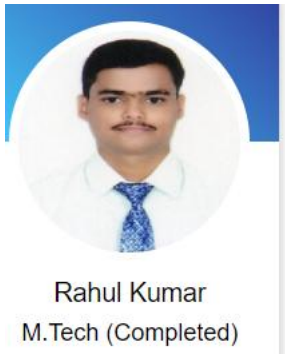
Anindya Kanti Roy
M.Tech (on-going)

Debanik Bose
M.Tech (completed)

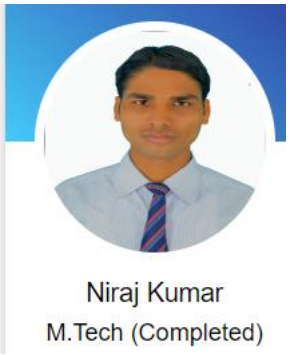


Sudeshna Gun
B.Tech-M.Tech Dual Degree (Completed)

Arghya Singha Mahapatra
M.Tech (completed)



Rahul Kumar
M.Tech (Completed)

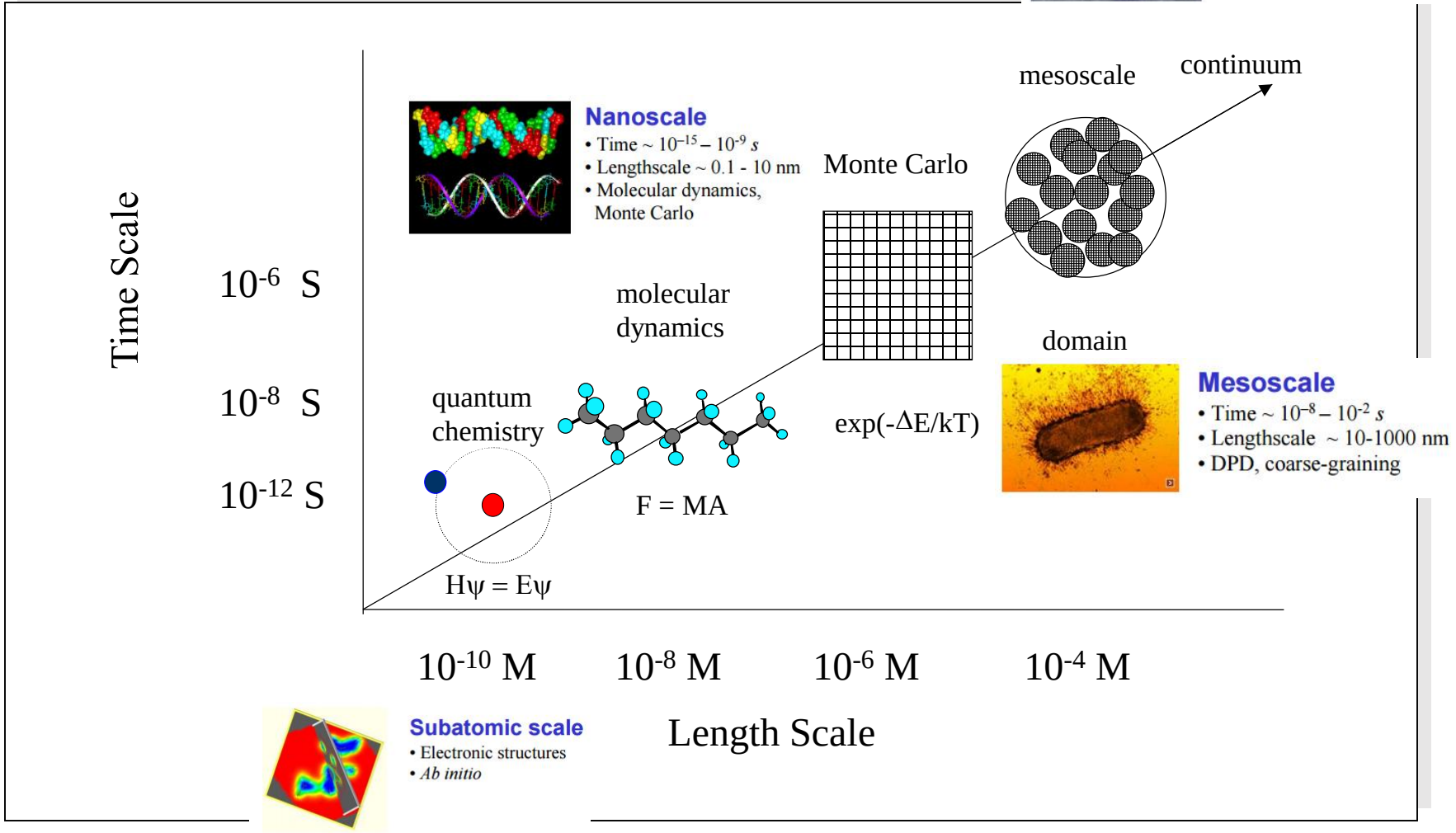


Niraj Kumar
M.Tech (Completed)

Background :

Scales in Simulations

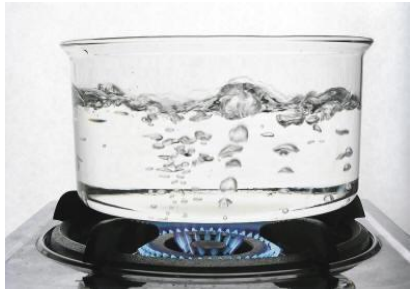
Macroscale
- Time > 1 *s*
- Lengthscale > 1μ
- Phase field models, FEM



Taken from Grant D. Smith
Department of Materials Science and Engineering
Department of Chemical and Fuels Engineering
University of Utah
http://www.che.utah.edu/~gdsmith/tutorials/tutorial1.ppt

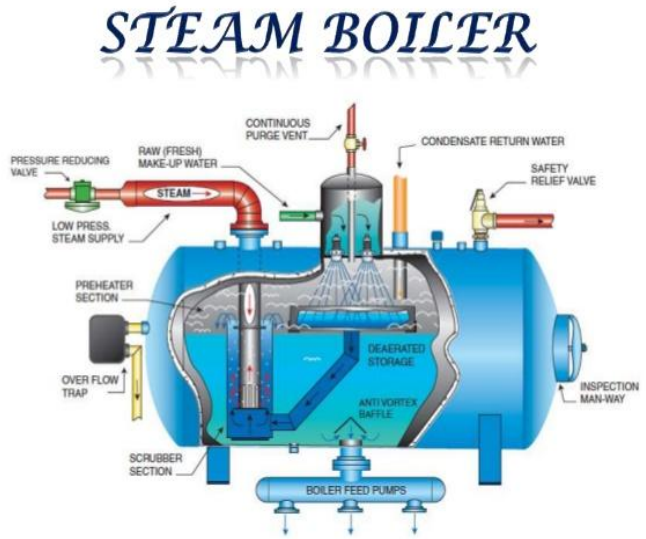
Boiling – an important Phase Change Process

❑ **Definition: Boiling is a phase change process with formation of vapor bubbles from liquid on a heated surface or in a superheated liquid layer adjacent to the heated surface. It is different from evaporation since it involves formation of liquid-vapor interface at discrete sites on the heated surfaces.**



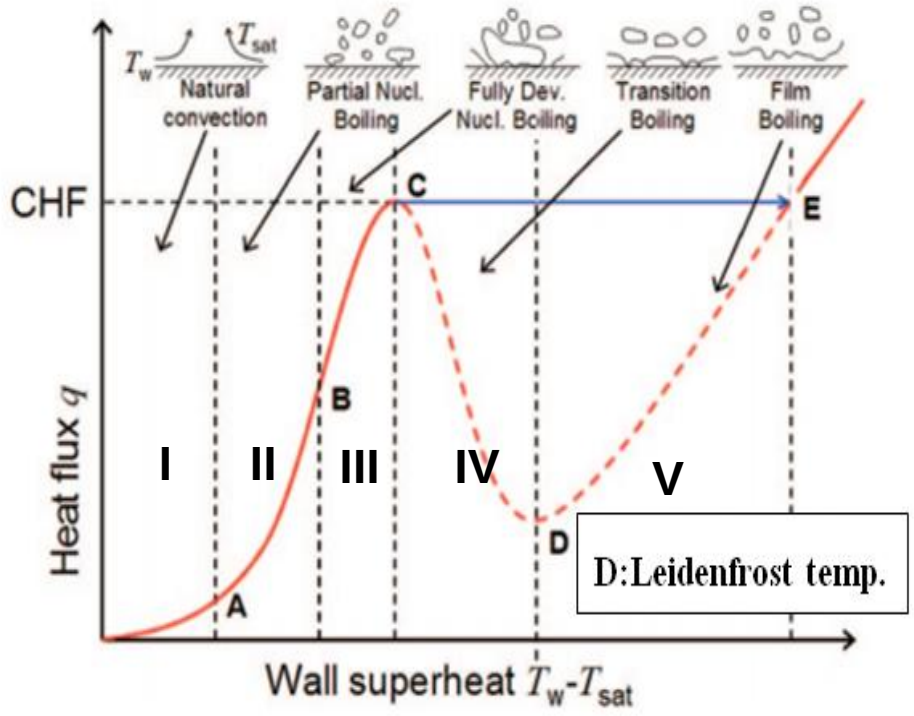
❑ **Applications**

- **Energy conversions**
- **Refrigeration and air conditioning**
- **Chemical thermal processing**
- **Microelectronic cooling**
- **Nuclear engineering**
- **Micro scale devices (MEMS, MTMS, sensors, micro heat pipes, biochips or lab-on-chips etc)**



Boiling! A complex phenomena to analyze mathematically

- ❑ Interaction of several parameters associated with heater and fluid .
- ❑ Mutiscale nature of the phenomena makes boiling a difficult problem to analyze.
- ❑ Based on the historic work of Nukiyama [1934], a qualitative boiling curve is established which gives us important understanding of different phases of boiling.



Qualitative boiling curve

Different regimes of boiling:

a. Natural convection region
b. Partial nucleate boiling region
c. Fully developed nucleate boiling region
d. Transition boiling region
e. Film boiling region

Ref: V. P. Carey, *Liquid-Vapor Phase Change Phenomena; Hemisphere Publishing* Corporation: New York. (1992)

Approaches to Analyze Film Boiling

- **Experiments: difficult due to**
  - **Small scales**
  - **Highly dynamic situation**
  - **two phases**

- **Semi-mechanistic models:**
  - **Existing correlations are based on questionable assumptions**
  - **Detailed physical understanding needed**

- **Numerical Simulations:**
  - **Accurate simulations give deeper insight into the physics**
  - **Can lead to better theoretical models**

Different Numerical Methods

Moving Grid or Lagrangian Methods: grid points are embedded with the fluid and moves with it

- Grid is Adaptive
- Points on interface are advected
- Interface reconstruction through advected points
- Interface boundary condition can be easily applied on the exact material interface

Disadvantages:

Fails when the fluid undergoes large distortions

Fix Grid or Eulerian Method: the mesh is treated as a fixed reference frame through which the fluid moves. e.g. VOF, LS, MAC methods

- Can handle extreme arbitrary distortions of fluid
- Fluid under interface is advected
- New interface is approximated by using volume fraction variable
- Can be applied easily to the domain with complex geometry

Disadvantages:

Free surfaces looses their intrinsic nature of sharp discontinuity

Interfacial instability plays an important role in film boiling.
Hence, accurate tracking of interface is essential

Interface Tracking Algorithms: Level Set (LS) and Volume of Fluid (VOF)

Level set Method (Osher and Sethian (1988))

• Interface is represented by a signed distance function (Φ), i.e.,

Φ > 0 in the liquid region,

Φ < 0 in the vapor region, and,

Φ = 0 at interface.

• The new Φ field is updated by solving an advection equation.

Advantages

• Accurate results for flows with high density differences

• Accurate calculation on unit normal and curvature of the interface.

Disadvantages

- Mass conservation not satisfied

Volume of Fluid (VOF) (Hirt and Nichols (1979))

- The method tracks volume fraction of each fluid in cells that contains portions of the interface, rather then the interface itself.

  Variable: liquid void fraction,

$$\alpha = \frac{\rho - \rho_g}{\rho_l - \rho_g}$$

$\alpha = 0$ Vapor

$\alpha = 1$ Liquid

$0 < \alpha < 1$ Two phase

- At each time step interface is reconstructed solving advection equation
- Update the void fractions for next time step

Advantages

- Liquid - vapor interface is captured explicitly
- Satisfies mass conservation

Disadvantages

- Not very accurate for flows with high density differences

Coupled Level Set Volume of Fluid (CLSVOF)

The CLSVOF (Sussman and Pucket (2000)) is an attempt to combine the advantages of the level-set and volume-of-fluid approaches.

- VOF advection algorithm is applied since it is mass conserving
- LS function is computed additionally to calculate the normal and curvature of the interface accurately
- Smoothness of the LS function helps to use simple finite-differencing scheme
- On the basis of the above reconstructed interface, the level-set function are redistanced to achieve mass conservation

Formulation of Saturated Film boiling

Governing Equations for Continuum Simulations

$$\int_{s_C} \vec{v}\,.\vec{n}\,ds + \int_{s_I(t)} \left(\frac{1}{\rho_l} - \frac{1}{\rho_g}\right)\frac{\|q\|.\vec{n}}{h_{lg}} = 0$$

$$\rho(\tilde{\alpha})\left(\frac{\partial \vec{v}}{\partial t} + \vec{v}.\nabla\vec{v}\right) = -\nabla p + \rho(\tilde{\alpha})\,\vec{g} + \nabla.\left\{\mu(\tilde{\alpha})\left[\nabla\vec{v} + (\nabla\vec{v})^T\right]\right\} + \sigma k \nabla\tilde{\alpha}$$

$$\rho c_p\left(\frac{\partial T}{\partial t} + \vec{v}.\nabla T\right) = \nabla.(k\nabla T)$$

Properties of liquid and vapor phases of water at near critical pressure

Water near critical: T_{sat} = 646 K; P_{sat} = 21.9 MPa; h_{lg} = 276.4 kJ/kg

σ = 0.07 mN/m

	Density(ρ) (kg/m^3)	Viscosity (μ) (μN s/m^2)	Conductivity(K) (mW/mK)	Specific heat(c_p) (KJ/kg K)
Liquid	402.4	46.7	545	2.18 X 10^2
Vapor	242.7	32.38	538	3.52 X 10^2

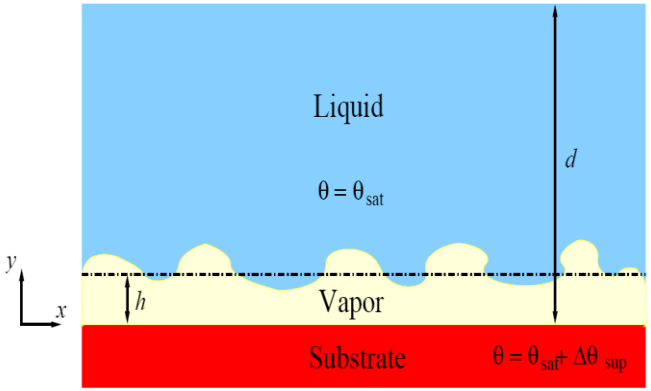
Solution Techniques

- Staggered grid arrangement (MAC, Harlow and Welch (1965))
- The grid - mesh used for grid independent simulations is 1200×240 using 240 grid cells per λ_B
- Uniform grid spacing
- Finite difference discretization scheme
- Second order accuracy in space
- Convective terms in momentum equation are discritized by ENO scheme
- Convective terms in energy equation are discretized by QUICK scheme
- Strong coupling between continuity and energy equations
- Pressure equation is arranged according to linear algebraic system interface of Hypre which is an open source code for high performance parallel computations. BoomerAMG, a preconditioned solver of Hypre is employed to solve the pressure equation.
- A typical time step of $\Delta t = 2.5 \times 10^{-6} s$ was used.

Boundary conditions

- Computations are performed in a $5\lambda_B \times \lambda_B$ domain where $\lambda_B = 0.002275$ m

  At $x = 0$ and $x = 5\lambda_B$: $\dfrac{\partial v}{\partial x} = 0$ and $\dfrac{\partial \theta}{\partial x} = 0$



Computational domain

- Constant wall temperature condition is used on the solid vapor interface,

  At $y = 0$: $\theta = \theta_{sat} + \Delta\theta_{\sup}$

- Outflow boundary conditions are applied on the top surface of the domain,

  At $y = H = \lambda_B$: $\dfrac{\partial u}{\partial y} = \dfrac{\partial v}{\partial y} = \dfrac{\partial \theta}{\partial y} = 0$ and $P = P_0$

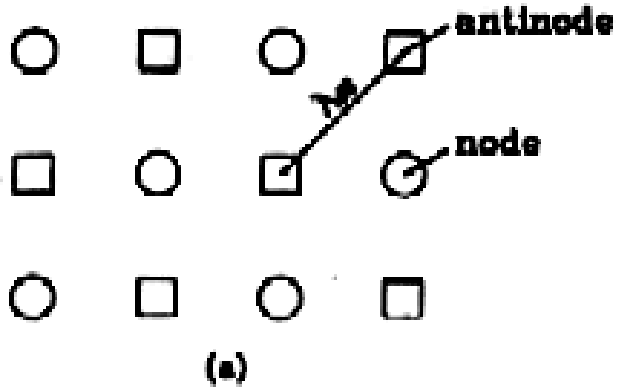
- The outlet pressure is taken to be the saturation pressure less the hydrostatic pressure difference from the initial film level to the outlet.

- The initial liquid - vapor interface is defined by assigning a random y location on the left and right faces of the fourth computational cell in the y-direction. The interface thus constructed consists of a range of wave numbers with arbitrarily assigned amplitudes.

Theoretical model

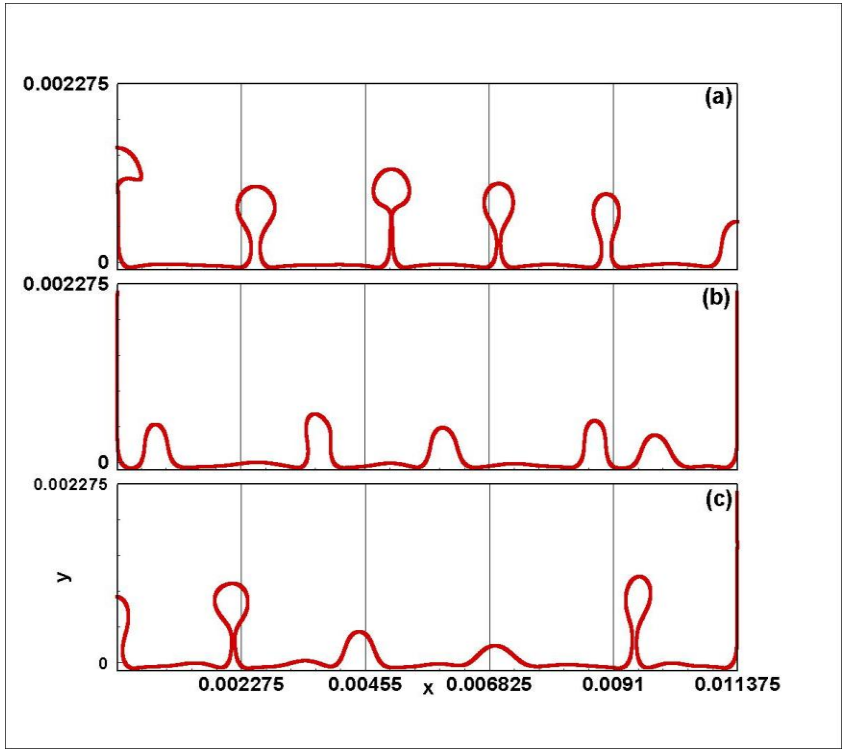
- **Berenson model** (1961) based on :
- 2D, horizontal surface
- Uniform film thickness
- Vapor bubbles are placed on a square grid with a spacing equal to the Taylor most dangerous wave length given as,

$$\lambda_B = 2\pi \sqrt{\frac{3\sigma}{(\rho_l - \rho_g)g}}$$



Important to note that T-H instability is based on potential flow and effect of viscosity is not considered.

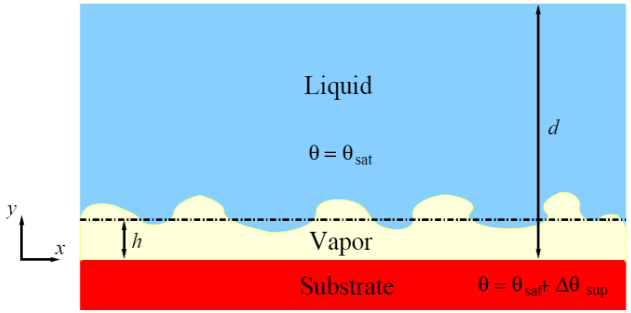
Our Results:



Interface profile for saturated water with Ja = 22.86 (ΔT = 18 K) and at an instant (a) 0.475 s, (b) 0.725 s, and (c) 0.925 s

Consecutive cycles of bubble Formation sites

Interfacial Instability in Film Boiling



Interfacial instability of film boiling

Rayleigh – Taylor instability
(when viscous force is dominant)

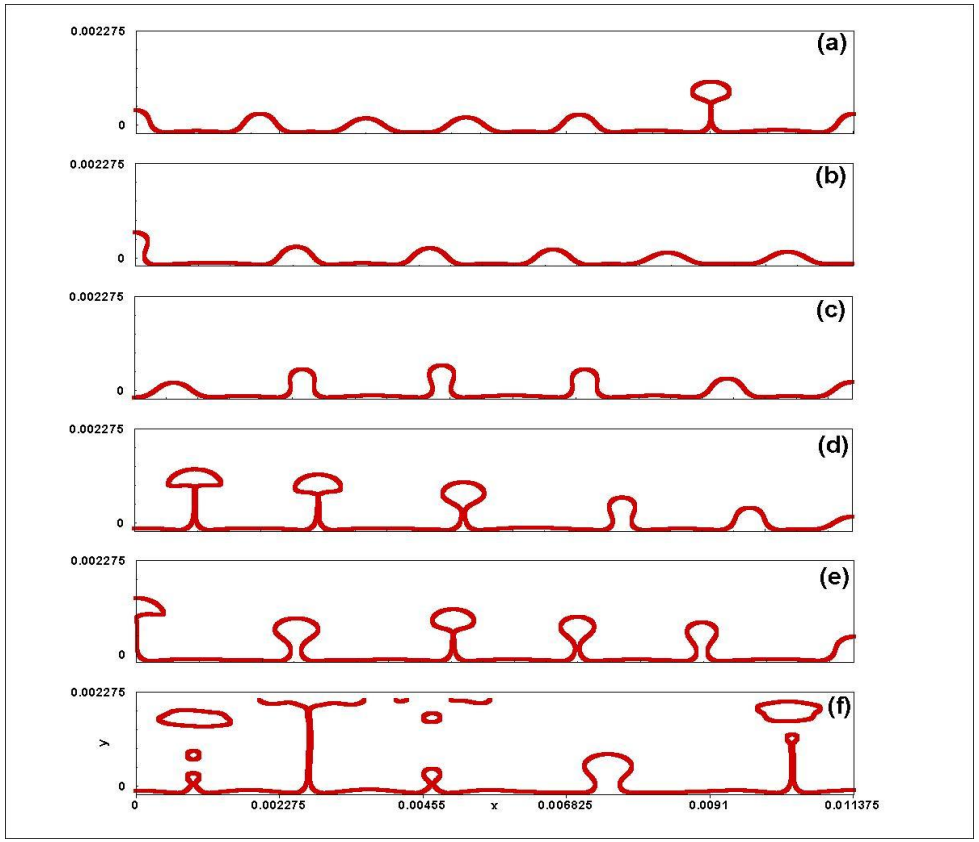
$$\lambda = 2\pi \sqrt{\frac{2\sigma}{\left(\rho_l - \rho_g\right)g}}$$

Taylor-Helmholtz instability.
(when viscous force is neglected)

$$\lambda_B = 2\pi \sqrt{\frac{3\sigma}{\left(\rho_l - \rho_g\right)g}}$$

Multimode analysis of bubble growth in $5\lambda_B \times \lambda_B$ domain

	Number of bubble formation sites
(a) Ja = 2.54 (ΔT = 2 K)	6
(b) Ja = 7.62 (ΔT = 6 K)	5.5
(c) Ja = 12.7 (ΔT = 10 K)	5.5
(d) Ja = 17.78(ΔT = 14 K)	5.5
(e) Ja = 22.86 (ΔT = 18 K)	5
(f) Ja = 25.4 (ΔT = 20 K)	5

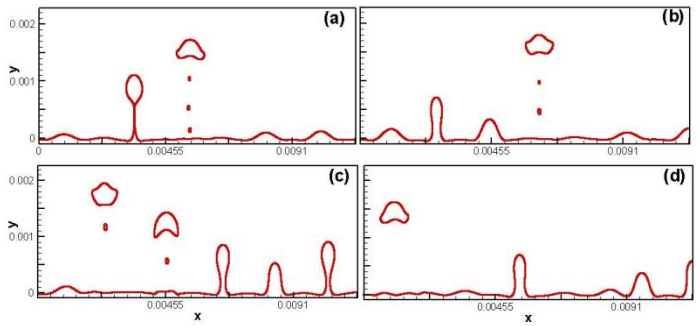


Transition from Rayleigh-Taylor to Taylor-Helmholtz instability

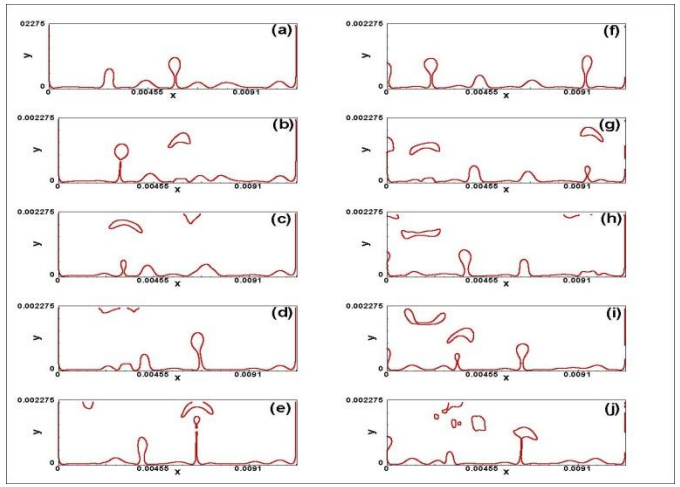
$$\lambda_B = 2\pi\sqrt{\frac{3\sigma}{(\rho_l - \rho_g)g}}$$

$$Ja = c_p \Delta\theta_{\text{sup}} / h_{\text{lg}}$$

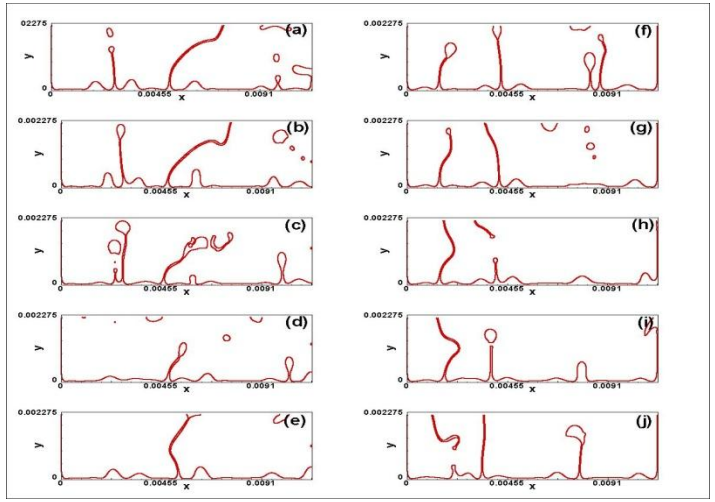
Different regimes of bubble formation in pool boiling:



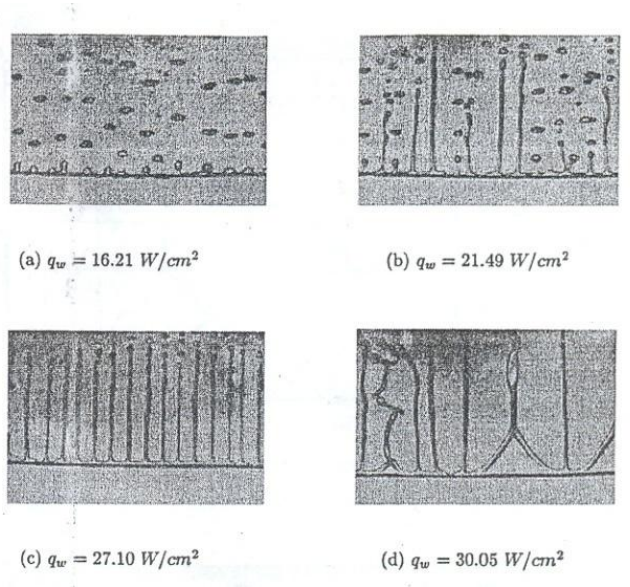
Laminar regime (ΔT = 2 – 6 K)



Turbulent regime (ΔT = 14 – 18 K)

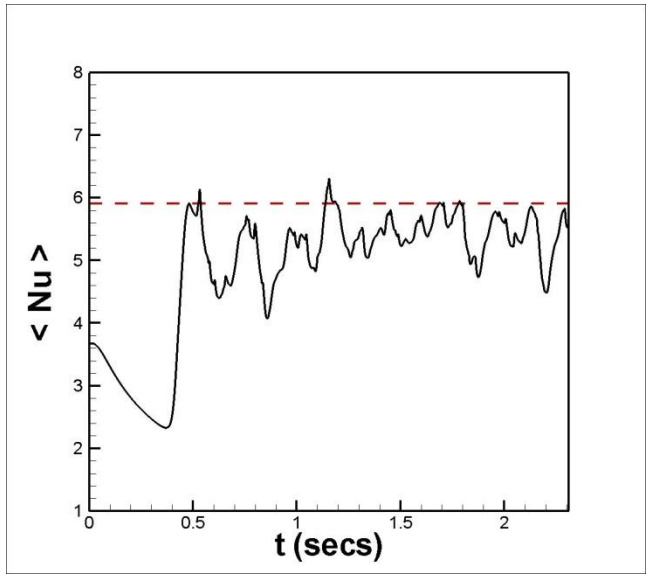


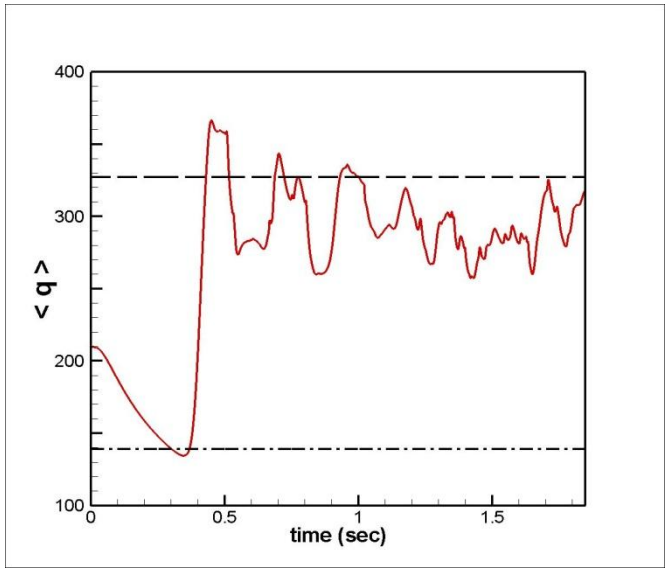
Column instability (ΔT = 20 – 22 K)



Experimental results of Reimann and Grigull (1975)

Variation of space-averaged Nusselt number and heat flux





Dotted lines show the analytical predictions of Nu, and maximum/minimum heat fluxes

$$Nu_{SD} = 0.265(Gr\,\mathrm{Pr})^{1/4}(Ja^{-1} + 0.5 + 1.3Ja^{1/4})^{1/4}$$

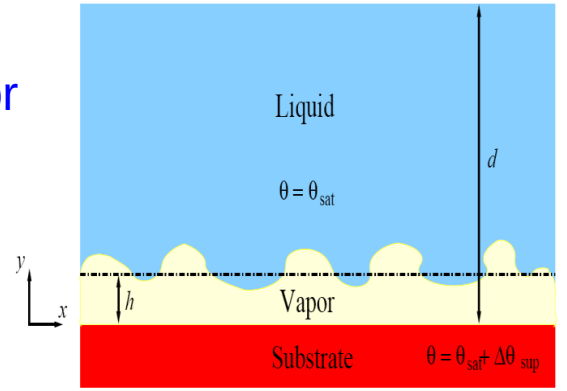
$$q_{\min} = 0.091\rho_g h_{fg}\left(\frac{\sigma g(\rho_l - \rho_g)}{(\rho_l + \rho_g)^2}\right)^{1/4} \qquad q_{\max} = \rho_g h_{fg}\frac{\pi}{16}\sqrt{\frac{4\sigma(\rho_l + \rho_g)}{\lambda\rho_l\rho_g}}\left[1 + \frac{\rho_g}{\rho_l}\frac{\pi}{(16-\pi)}\right]^{-1}$$

Reference: A. Hens *et al*., **Physics of fluids,** 26, 012105 (2014)

Limitation of Continuum Dynamics and Need of Molecular Level Study:

- In CD, we assumed the presence of a pre-existing vapor film on the heater surface

- Questions : **What is the origin of this vapor phase ?**
  How does this vapor phase appear ?



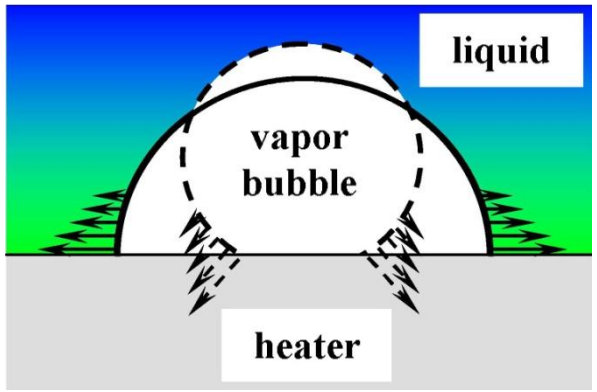
Computational domain of continuum study

- This vapor phase appears due to vapor bubble nucleation which is initiated from a phase change process at molecular level

- Extreme small time and length scale of this process makes it difficult to study experimentally

- Continuum models do not remain valid at such length scale

Molecular dynamics simulation offers an way out to investigate these phenomena

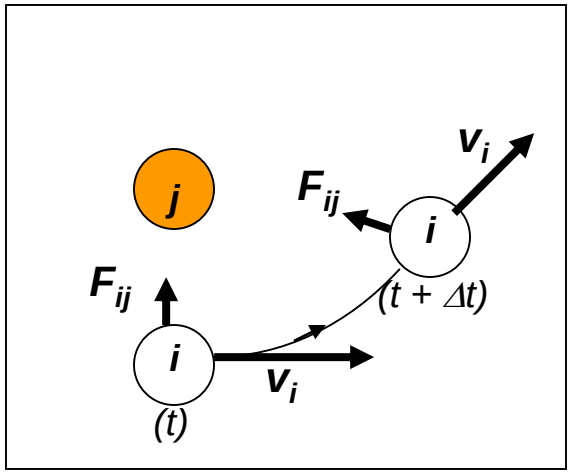


Schematic of vapor bubble nucleation

Molecular Dynamics

- Deterministic method.
- From atom positions, velocities and accelerations, calculate atom positions and velocities at the next time step.
- Integrating these infinitesimal steps yields the trajectory of the system for any desired time range

- Newton's Law $\sum_j \vec{F}_{ij} = m_i \frac{d\vec{v}_i}{dt}$ $\vec{F}_{ij} = -\frac{\partial \phi_{ij}}{\partial r_{ij}} \hat{r}_{ij}$



- Updated Position:

$$\vec{r}_i(t+\Delta t) = \vec{r}_i(t) + (\Delta t)\vec{v}_i(t) + \frac{1}{2}(\Delta t)^2 \frac{\vec{F}_i(t)}{m_i}$$

- Updated Velocity:

$$\vec{v}_i\left(t + \frac{\Delta t}{2}\right) = \vec{v}_i(t) + \frac{1}{2}(\Delta t)\frac{\vec{F}_i(t)}{m_i} \qquad \vec{v}_i(t+\Delta t) = \vec{v}_i\left(t + \frac{\Delta t}{2}\right) + \frac{1}{2}(\Delta t)\frac{F_i(t+\Delta t)}{m_i}$$

Basic idea:

- Initialize the system
- Move and integrate for several time steps

MD simulation of initial stages of vapor bubble nucleation

Classical molecular dynamics simulation is employed to investigate the initial stages of bubble nucleation

Simulation Detail:

System : A liquid argon film on solid platinum surface

Forcefield : Lennard-Jones (LJ) 12-6 potential is considered for all kind of inter atomic potential

$$\phi_{ll}(r) = 4\varepsilon_{ll}\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \qquad \phi_{wl}(r) = 4\varepsilon_{wl}\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \qquad \phi_{ww}(r) = 4\varepsilon_{ww}\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

Integration method: Velocity – Verlet

Ensemble : NVT for the overall system during equilibration stage and during production stage NVE is considered for liquid Ar and Pt surface is under NVT ensemble

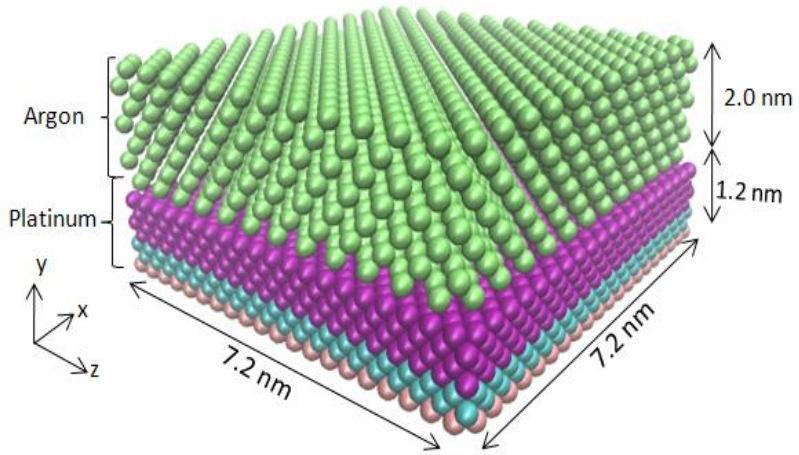
Thermostat : Nose – Hoover

Time step : 1 femto second

Cut off radius : 11.9 A

Package : LAMMPS (an open source code developed by Sandia National Laboratory, US)

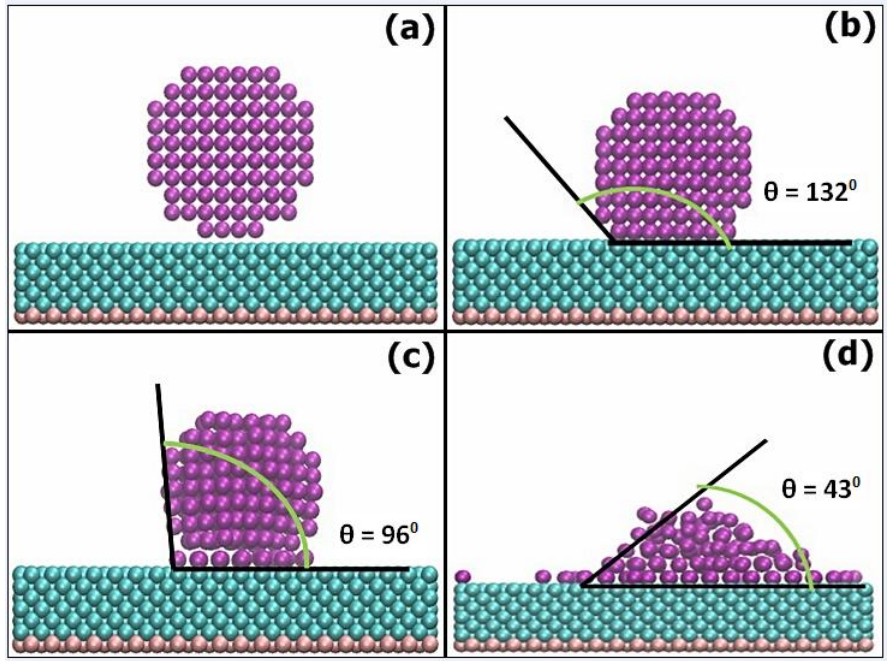
MD simulation……. Cont.



Initial configuration of the system with appropriate dimensions.

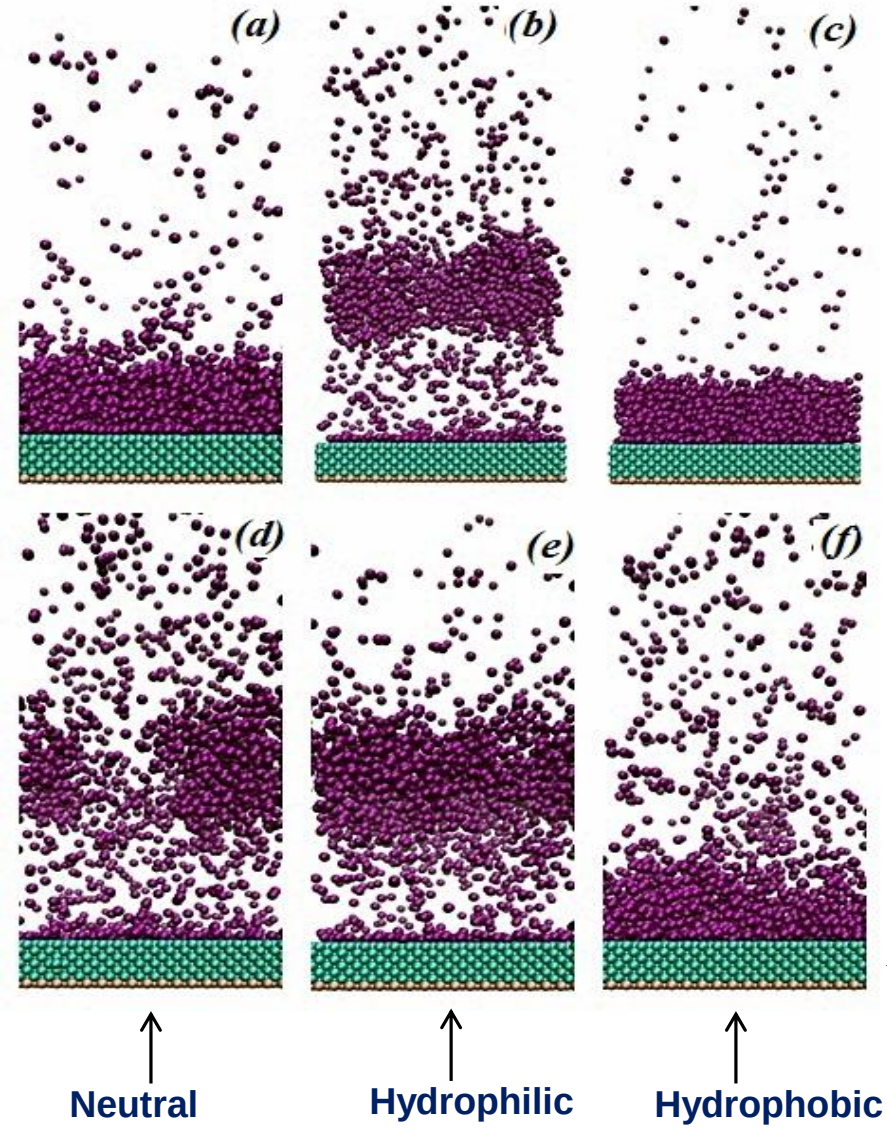
To study the effect of surface wettability on the boiling three different type of surfaces are considered by varying the solid-liquid interaction potential.

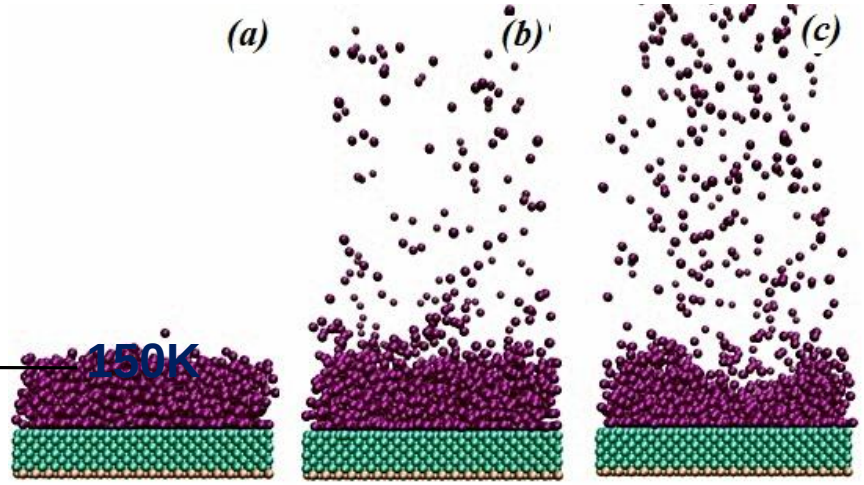
1. $\varepsilon_{ll} < \varepsilon_{wl}$, hydrophilic
2. $\varepsilon_{ll} > \varepsilon_{wl}$, hydrophobic
3. $\varepsilon_{ll} = \varepsilon_{wl}$, neutral



Solid liquid interface wettability and equilibrium contact angles (ɵ) of nanodroplet on solid surface: (a) initial state, (b) $\varepsilon_{ll} > \varepsilon_{wl}$ or $\varepsilon_{ll}/\varepsilon_{wl}=2$ ($ɵ=132^0$ and hydrophobic), (c) $\varepsilon_{ll} = \varepsilon_{wl}$ or $\varepsilon_{ll}/\varepsilon_{wl}=1$ ($ɵ=96^0$ and neutral), (d) $\varepsilon_{ll} < \varepsilon_{wl}$ or $\varepsilon_{ll}/\varepsilon_{wl}=0.2$ ($ɵ=43^0$ and hydrophillic)

MD simulation……. Cont.





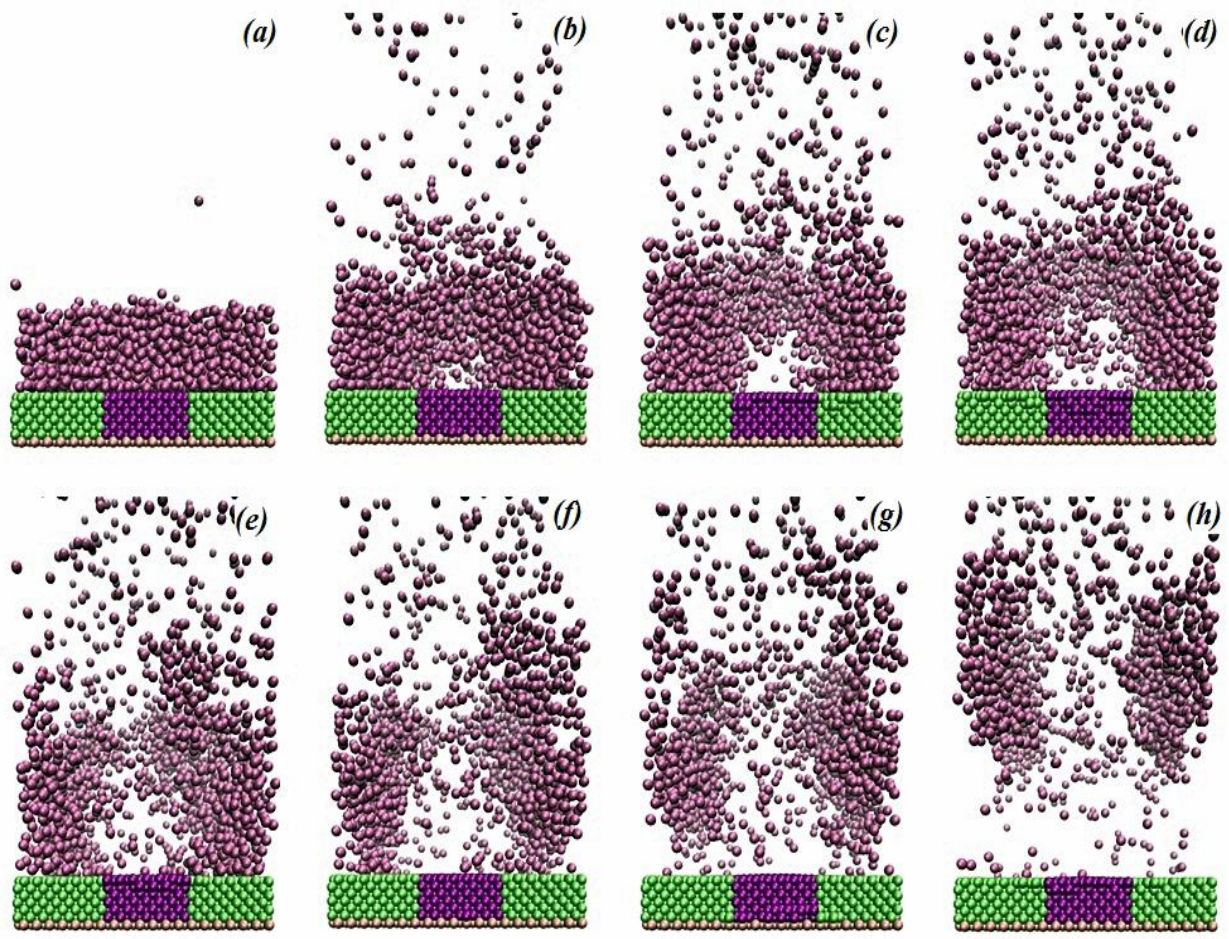
Evaporation on uniformly heated wall at 90K. (a) - (c) is showing the side view of systems at 0 ps, 50 ps and 100 ps respectively.

Hydrophilic surface facilitates heat transfer

250K

Boiling on uniformly heated wall at 150K [(a) - (c)] and at 250K [(d) - (f)]. (a),(d) are showing the snapshots when the surface is of neutral wettability whereas (b), (e) and (c),(f) are the cases when the surface is hydrophilic and hydrophobic respectively.

MD simulation……. Cont.

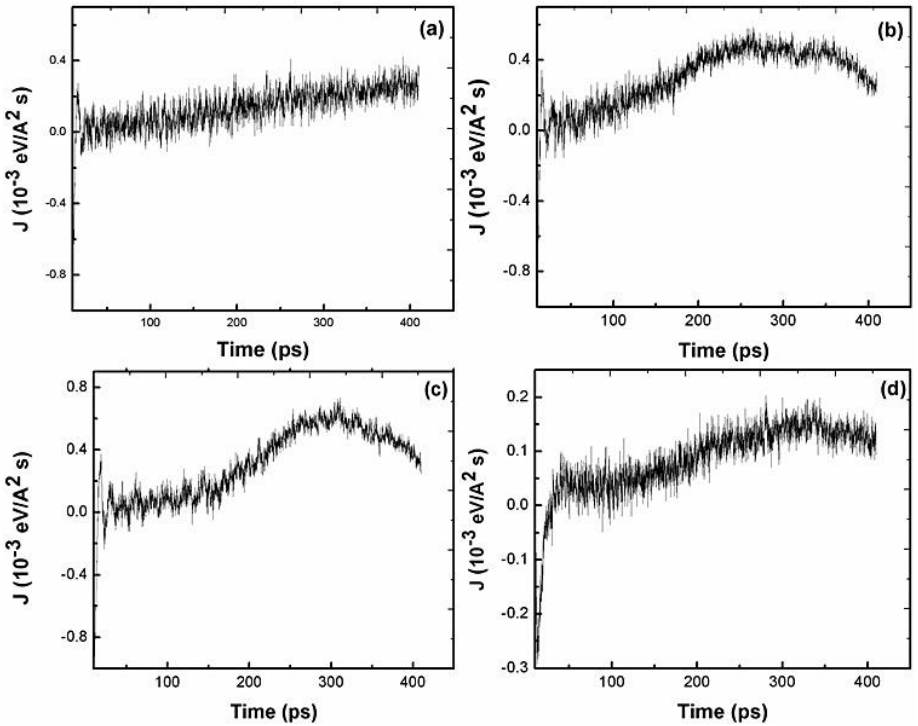


Nucleate boiling on partially heated wall where the middle part of the surface is at 500K and both sides of the surface is at 150K. Snapshots (a) to (h) are showing the time evolution of the system which are taken at 0 ps, 40 ps, 48 ps, 52 ps, 56 ps, 60 ps, 64 ps and 74 ps respectively.

MD simulation……. Cont.

$$q_{max} = \rho_g h_{fg} \sqrt{RT/2\pi}$$

- ✓ Equation of heat flux from Kinetic theory which predicts 10^8 W/m^2
- ✓Normal experimental result shows heat flux in the order of 100 W/m^2



Our results show the heat flux in the order of 10^8 W/m^2

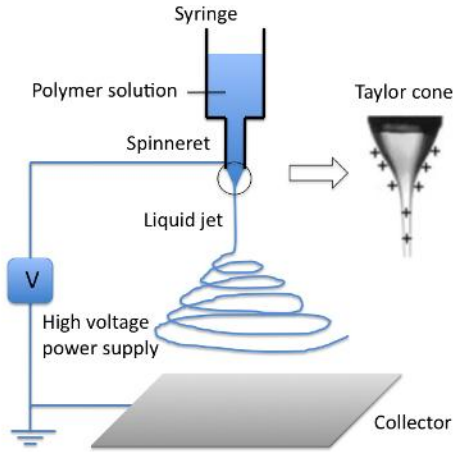
Profile of heat flux normal to the surface at the liquid film for a specific type of case 1 when the surface temperature is 150K (a); for a particular type of case 2 when the surface is of neutral wettability and its temperature is 250K (b); a particular type of case 3 when the middle portion of the hydrophobic surface is at 500K and the sides are at 150K (c); a particular type of case 4 when the patterned surface is at a temperature of 150K (d).

Reference: A. Hens *et al.*, **International Journal of Heat and Mass Transfer**, 71, 303 (2014)

Nano-droplet evaporation in presence of external electric field

Interaction between external electric field and water droplet forms the basis of many microelectronic and nano-optoelectronic technologies such as:

- **Electrospinning**
- **Electrospraying**
- **Nanoimprinting**
- **Electrostatic painting etc.**



In most of these applications water is used as solvent. So, understanding the mechanism of water droplet evaporation at nano-scale is necessary.

Models and methodology

For water-water interaction SPC/E model is considered

$$U_{nonbonded} = 4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r}\right)^{12} - \left(\frac{\sigma_{ij}}{r}\right)^{6}\right] + \frac{q_i q_j}{4\pi\varepsilon_0 r_{ij}}$$

For Pt-Pt interaction EAM model is considered

$$E_i = F\left(\sum_{j\neq i}\rho(r_{ij})\right) + \frac{1}{2}\sum_{j\neq i}\phi(r_{ij})$$

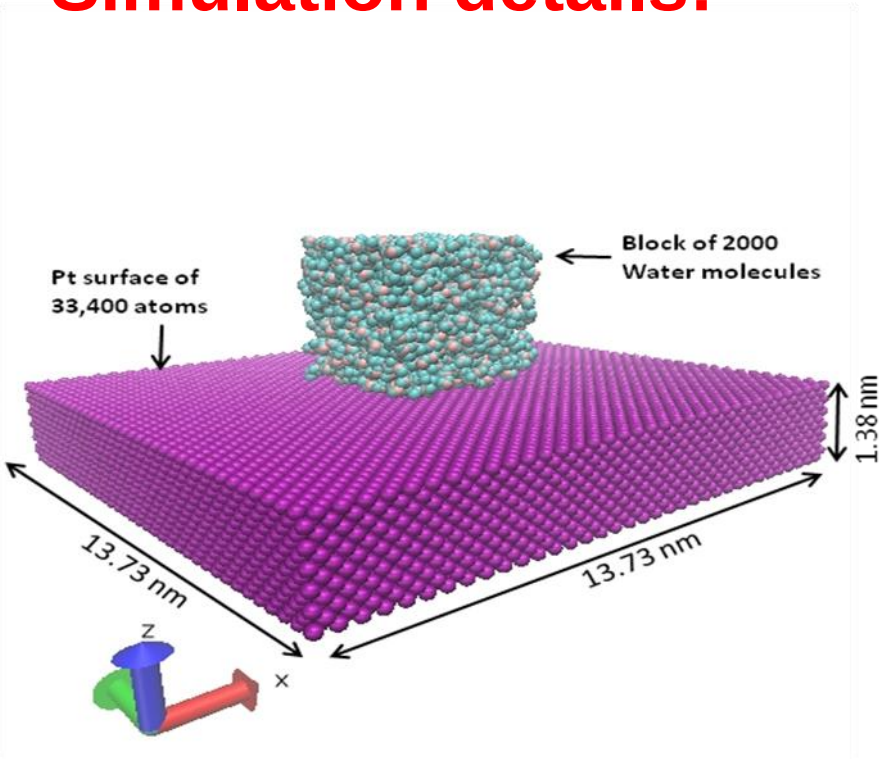
For water-Pt interaction Lennard-Jones model with DFT parameters is considered

$$U_{ls}(r_{ij}) = 4\varepsilon_{ls}\left[\left(\frac{\sigma_{ls}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ls}}{r_{ij}}\right)^{6}\right]$$

Energy contribution from applied electric field is given by

$$U_{field} = -\sum_{i=1}^{N}\sum_{k=1}^{3} q_k\,(r_k^{\,i}\cdot E)$$

Simulation details:



Initial structure of Pt-water system

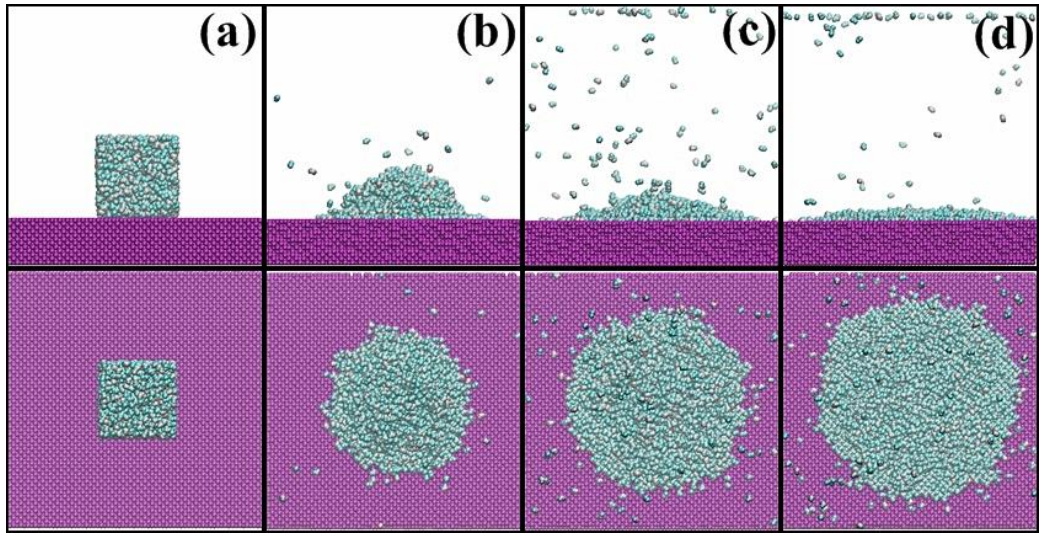
Time step: 1 femtosecond

Ensemble: NVT/NVE

Thermostat: Nose-Hoover

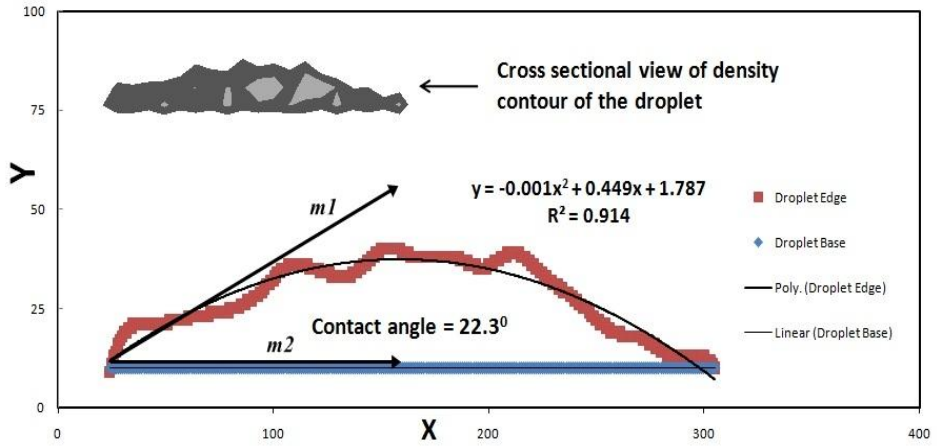
Damping constant: 0.1ps

Spreading of water droplet on Pt surface (validation of the model parameters)

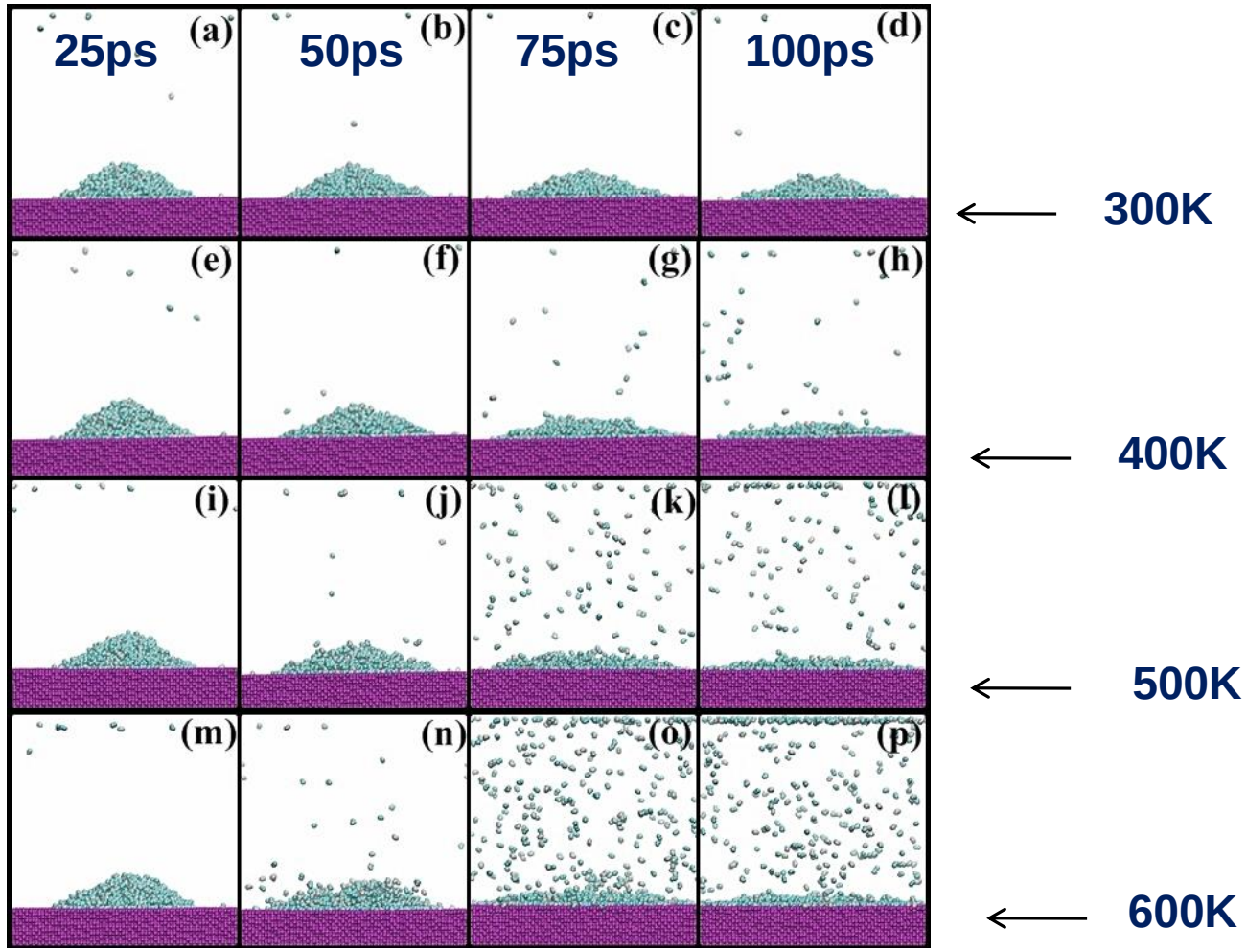


Temporal evolution of water droplet on Pt surface. (a) shows initial state of the water block. (b) and (c) show the images of the droplet after 25 and 50 ps respectively during heating the system to a temperature of 320 K. (d) shows the image of the final state of the droplet after keeping the system isothermally at 320K for 50 ps (after the heating step). Images in the bottom row show the respective top views of the systems.

Determination of contact angle by edge detection followed by curve fitting. Contact angle is measured from the final state of the results at 320K

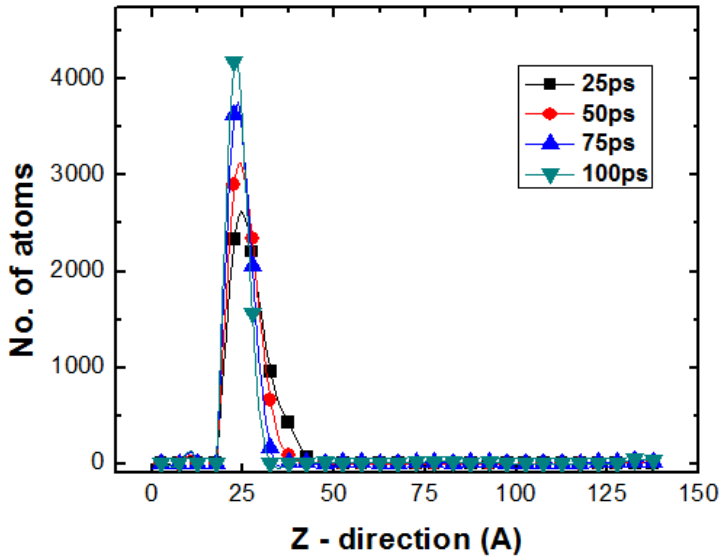


Evaporation of water droplet at different surface temperatures

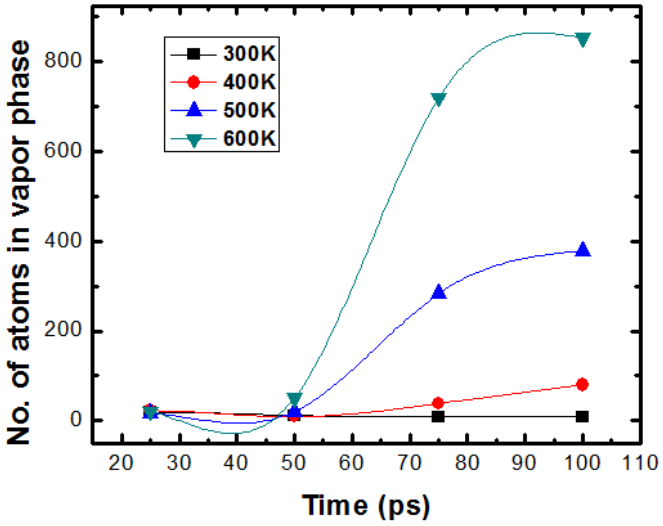


Effect of surface temperature on water droplet evaporation on Pt surface. Images in the 1st and 2nd column show the snapshots after 25 ps and 50ps respectively during surface heating from 100K to 300K (1st row), 400K(2nd row), 500K(3rd row) and 600K(4th row) respectively. Images in the 3rd and 4th row show the snapshots after 50 ps and 100ps respectively during isothermal surface heating at 300K (1st row), 400K(2nd row), 500K(3rd row) and 600K(4th row) respectively.

Cont..

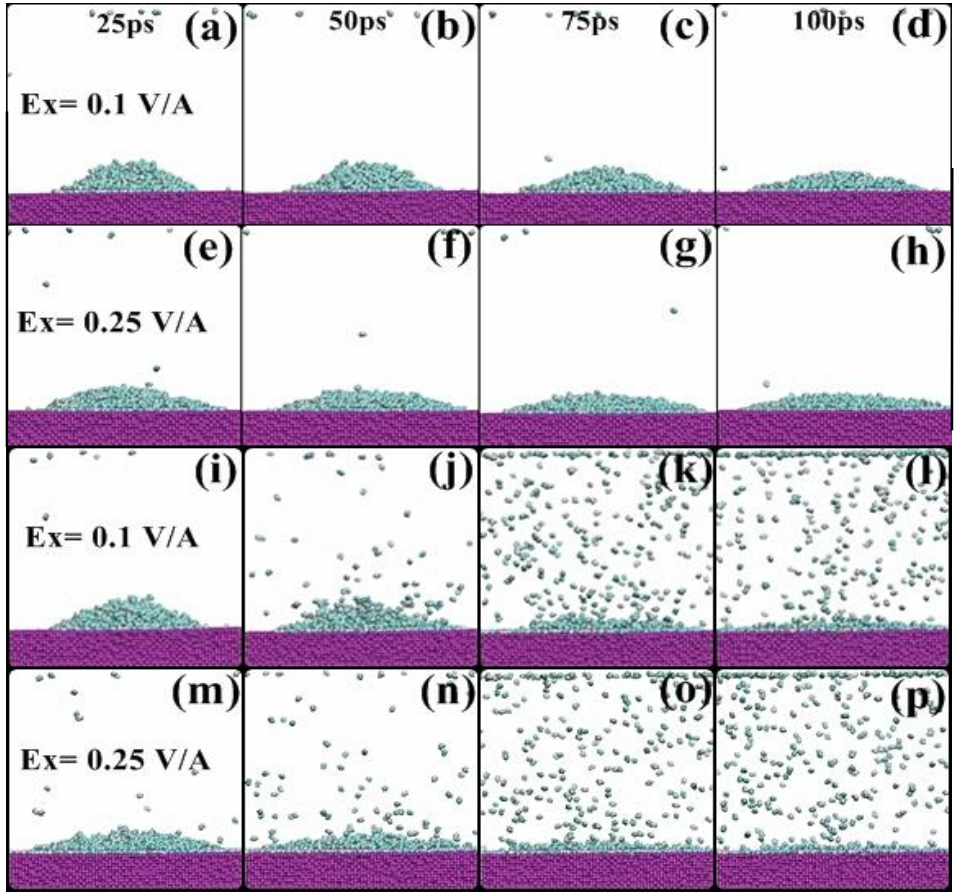


Variation of bin-wise number of atoms (of water molecules) along Z-direction.



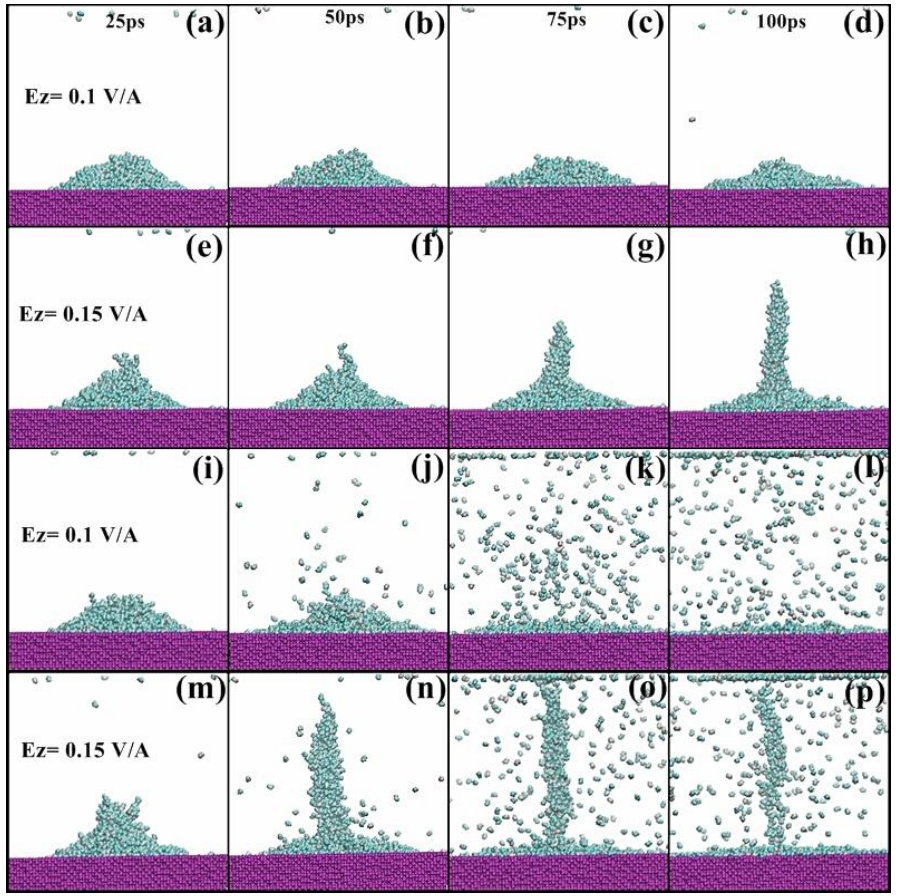
Variation of number of atoms (of water molecules) in vapor phase with time in absence of electric field at different substrate heating conditions.

Water droplet evaporation in presence of horizontal electric field



Effect of electric field in horizontal (X) direction on water droplet evaporation on Pt surface. Images in the 1st to 2nd column show the snapshots after 25 ps and 50ps respectively during surface heating from 100K to 300K (600K for 3rd and 4th row). Images in the 3rd and 4th column show the snapshots at 75 ps and 100ps respectively during isothermal surface heating at 300K (600K for 3rd and 4th row). In 1st and 3rd row, applied electric field is 0.1 V/Å whereas in 2nd and 4th row, applied electric field is 0.25 V/Å.

Water droplet evaporation in presence of vertical electric field



Effect of electric field in vertical (Z) direction on water droplet evaporation on Pt surface. Images in the 1st to 2nd column show the snapshots after 25 ps and 50ps respectively during surface heating from 100K to 300K (600K for 3rd and 4th row). Images in the 3rd and 4th column show the snapshots at 75 ps and 100ps respectively during isothermal surface heating at 300K (600K for 3rd and 4th row). In 1st and 3rd row, applied electric field is 0.1 V/Å whereas in 2nd and 4th row, applied electric field is 0.15 V/Å.

Relevant publications on droplet and bubble dynamics

1. Probir Biswas, Raj Agarwal, Braj Bhushan, Abhiram Hens*, Gautam Biswas*, “Interfacial hydrodynamics of electrosprays using leaky dielectric fluids", **Physics of Fluids**, Vol. 37 (2025)
2. Indradev Kumar, Sandip Kumar Lahiri, Abhiram Hens*, Gautam Biswas*, “Influence of surface morphology and temperature on nanoscale boiling of liquid nitrogen on a platinum substrate”, **International Journal of Thermal Sciences**, Vol. 210, pp. 109655 (2025)
3. Indradev Kumar, Sandip Kumar Lahiri, Abhiram Hens*, “Heat transfer analysis of liquid nitrogen film boiling in the presence of reduced gravity and electric field”, **Numerical Heat Transfer, Part A: Applications**, (Accepted on 25th October, 2024)
4. Indradev Kumar, Anindya Kanti Roy, Abhiram Hens*, “Effect of pressure variations on film boiling characteristics of liquid nitrogen”, **Physics of Fluids,** Vol. 35, pp. 101102 (2023)
5. S. Chatterjee, I. Kumar, K. C. Ghanta, **A. Hens*,** G. Biswas*, “Insight into molecular rearrangement of a sessile ionic nanodroplet with applied electric field”, **Chemical Engineering Science**, Vol. 247, page. 117083 (2022)
6. S. Chatterjee, **A. Hens*,** K. C. Ghanta, G. Biswas*, “Molecular dynamics study of sessile ionic nanodroplet under external electric field”, **Chemical Engineering Science**, Vol. 229, page. 116143 (2021)
7. **A. Hens**, G. Biswas, S. De, "Evaporation of water droplet on Pt-surface in presence of external electric field - A molecular dynamics study", **Journal of Chemical Physics**, 143, 094702 (2015)
8. **A. Hens**, G. Biswas, S. De, "Analysis of interfacial instability and multimode bubble formation in saturated boiling using coupled level set and volume-of-fluid approach", **Physics of Fluids**, 26, 012105 (2014)
9. **A. Hens**, R. Agarwal, G. Biswas, "Nano-scale study of boiling and evaporation in liquid Ar film on a Pt -heater using molecular dynamics simulation", **International Journal of Heat and Mass Transfer**, 71, 303 (2014)

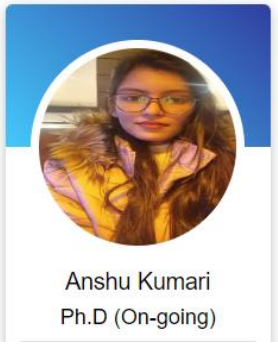
Acknowledgement

- **My Students**
- **My Colleagues and collaborators**
- **My Institute (NIT Durgapur)**

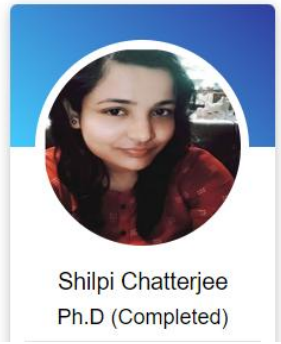
Thank You!

My Students

Braj Bhushan
Ph.D (on-going)

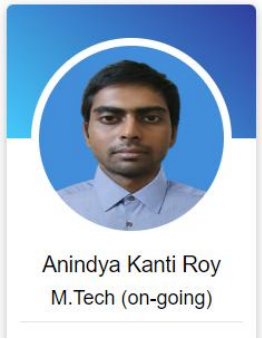


Anshu Kumari
Ph.D (On-going)

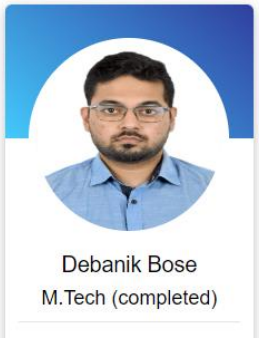


Shilpi Chatterjee
Ph.D (Completed)

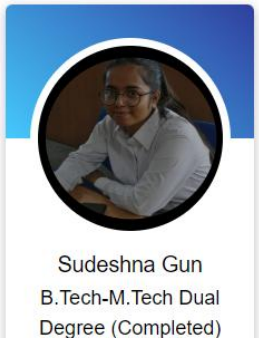
Indradev Kumar
Ph.D (Ongoing)



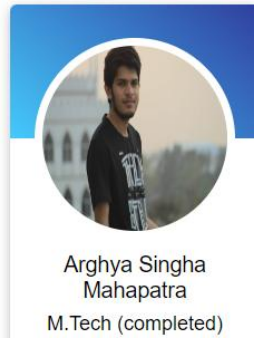
Anindya Kanti Roy
M.Tech (on-going)



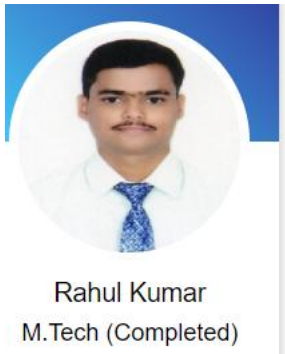
Debanik Bose
M.Tech (completed)



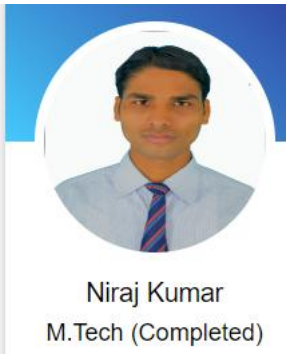
Sudeshna Gun
B.Tech-M.Tech Dual Degree (Completed)



Arghya Singha Mahapatra
M.Tech (completed)



Rahul Kumar
M.Tech (Completed)



Niraj Kumar
M.Tech (Completed)