AFRL-MN-EG-TP-2007-7407

SIMULATING THE DYNAMICS OF PARTICLES INTERACTING WITH SOLIDIFICATION FRONTS (PREPRINT - BRIEFING CHARTS)

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JULY 2007

CONFERENCE PAPER PREPRINT (BRIEFING CHARTS)

This paper will be presented at the 9th U.S. National Congress on Computational Mechanics, 23-26 July 2007, San Francisco, CA. One of the authors is a U.S. Government employee working within the scope of his position; therefore, the U.S. Government is joint owner of the work. If published, the publisher may assert copyright. If so, the U.S. Government has the right to copy, distribute, and use the work by or on behalf of the U.S. Government. Any other form of use is subject to copyright restrictions.

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- **Air Force Materiel Command**
- **United States Air Force**
- **Eglin Air Force Base**

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*
XX-07-2007

2. REPORT TYPE
CONFERENCE PAPER PREPRINT

3. DATES COVERED *(From - To)*

4. TITLE AND SUBTITLE
SIMULATING THE DYNAMICS OF PARTICLES INTERACTING WITH SOLIDIFICATION FRONTS (PREPRINT - BRIEFING CHARTS)

5a. CONTRACT NUMBER
N/A

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER
62602F

5d. PROJECT NUMBER
2502

5e. TASK NUMBER
07

5f. WORK UNIT NUMBER
37

6. AUTHOR(S)
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7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

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Munitions Directorate
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Eglin AFB, FL 32542-6810

2. Falk Corp.
Milwaukee, WI

3. The Univ. of Iowa
Iowa City, IA

8. PERFORMING ORGANIZATION REPORT NUMBER
AFRL-MN-EG-TP-2007-7407

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

Air Force Research Lab.
Munitions Directorate
AFRL/MNAC
Eglin AFB, FL 32542-6810

10. SPONSOR/MONITOR'S ACRONYM(S)
AFRL-MN-EG

11. SPONSOR/MONITOR'S REPORT NUMBER(S)
SAME AS BLOCK 8

12. DISTRIBUTION/AVAILABILITY STATEMENT
DISTRIBUTION A: Approved for public release; distribution unlimited.
Approval Confirmation #AAC/PA 06-07-07-448; dated 7 June 2007.

13. SUPPLEMENTARY NOTES
This paper will be presented at the 9th U.S. National Congress on Computational Mechanics, 23-26 July 2007, San Francisco, CA. One of the authors is a U.S. Government employee working within the scope of his/her position; therefore, the U.S. Government is joint owner of the work. (*Cont. on abstract below)

14. ABSTRACT

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Abstract:
1. Developed a multiscale numerical approach to solve particle-solidification front problems in a general manner
2. Model can be generalized to solve a variety of problems involving interacting interfaces
3. First to look at the physics from a nonlinear dynamics point-of-view (i.e. phase-space point of view)
4. Model captures essential physics that past research has neglected

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			JUSTIN GARVIN
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	SAR	48	**19b. TELEPHONE NUMBER** *(Include area code)*

Simulating the Dynamics of Particles Interacting with Solidification Fronts

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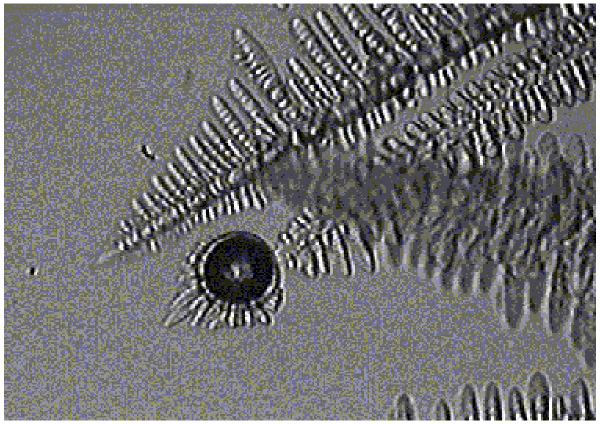
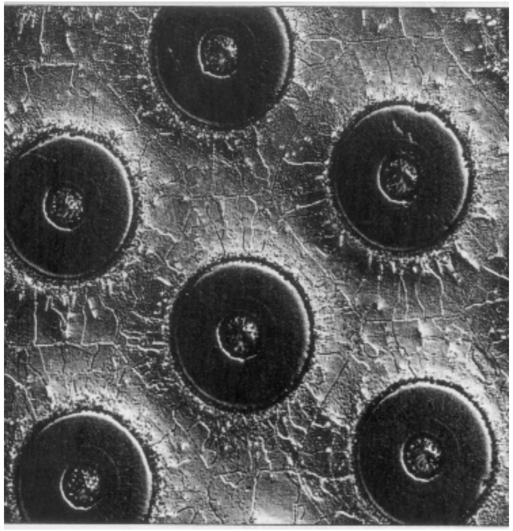
Motivation

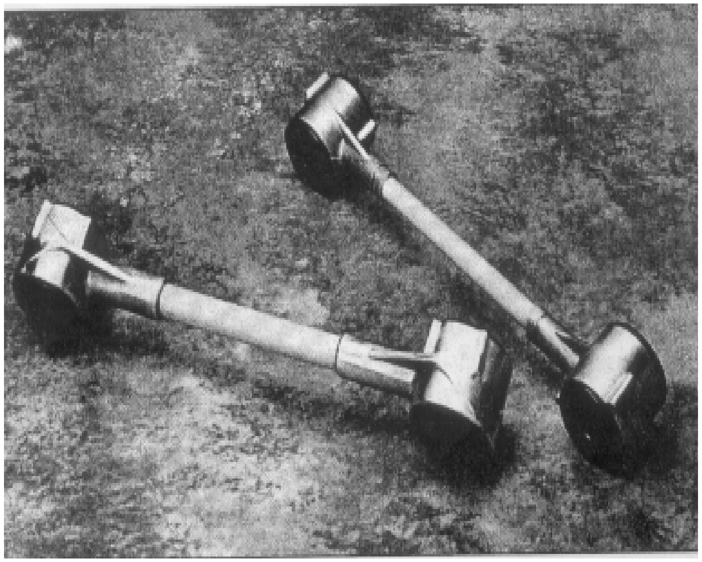
- Particle-solidification front interactions play a crucial role in predicting microstructures of metal-matrix composites (MMCs)



MMCs: Micron-sized particles embedded in a metal matrix – acts as reinforcement

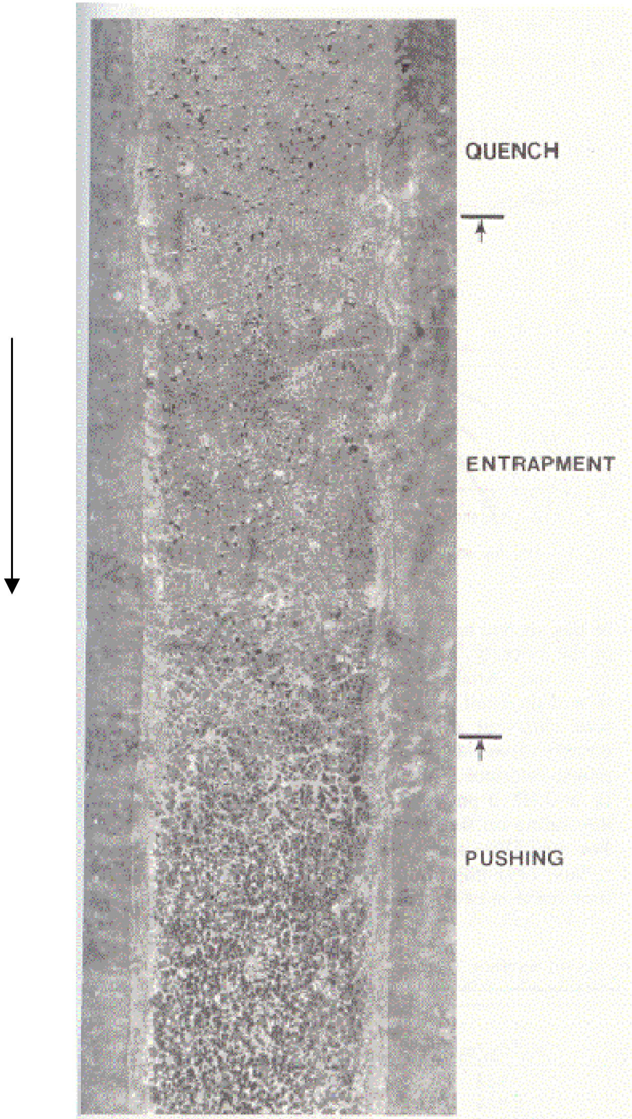
Industies: Automotive, aerospace
Properties: lightweight, good wear resistance



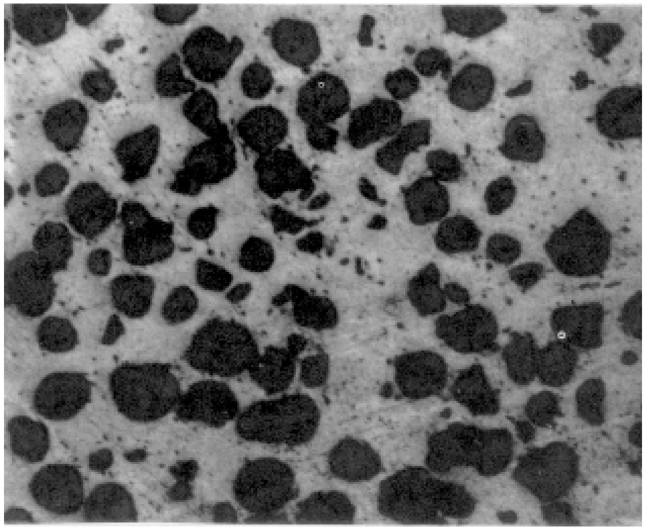


Processing of MMCs

Directionally solidified Al-17Cu/SiC. 21x



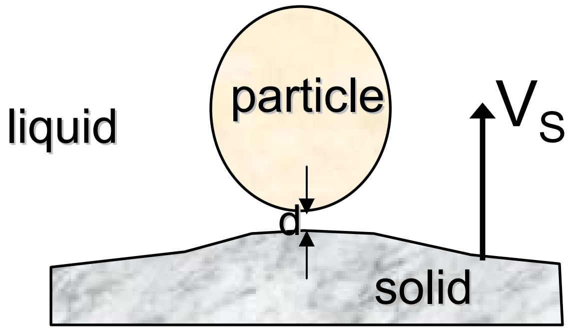
As-cast Al-2Mg/20 wt pct graphite. 31x



Want: Uniform distribution of particles
Need: Understand particle-front interactions

What happens when a solidification front interacts with a particle?

- As solidifying front approaches a particle it will either be
  - Engulfed
  - Pushed
  - Pushed, then engulfed



- Critical velocity, V_{CR}
  - Solidification velocity, $V_s \le V_{CR}$ → particle pushing
  - $V_s > V_{CR}$ → particle engulfment

♦ **Challenge**: A multiscale model that couples the dynamics in the gap with the overall thermal/fluid transport

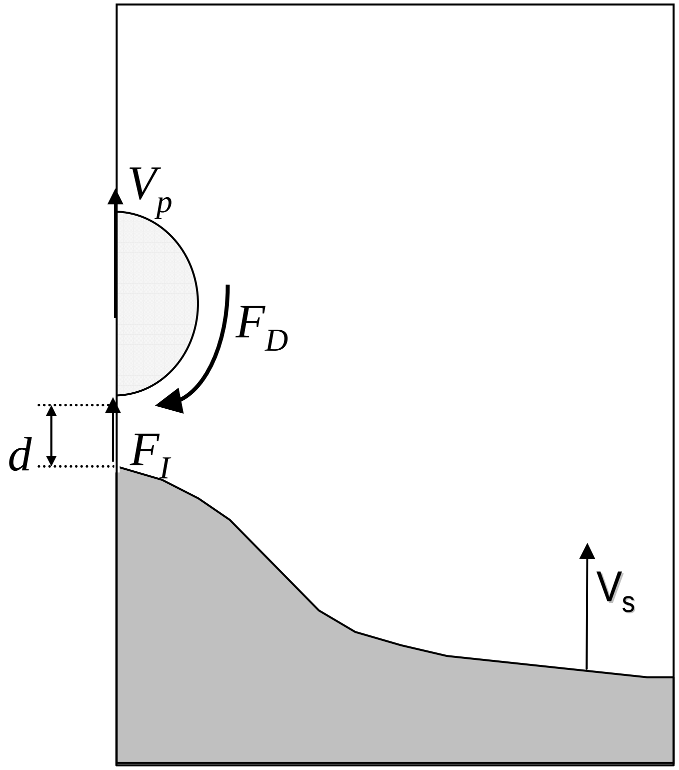
Physics of particle-solidification front interactions

Dynamics of the particle

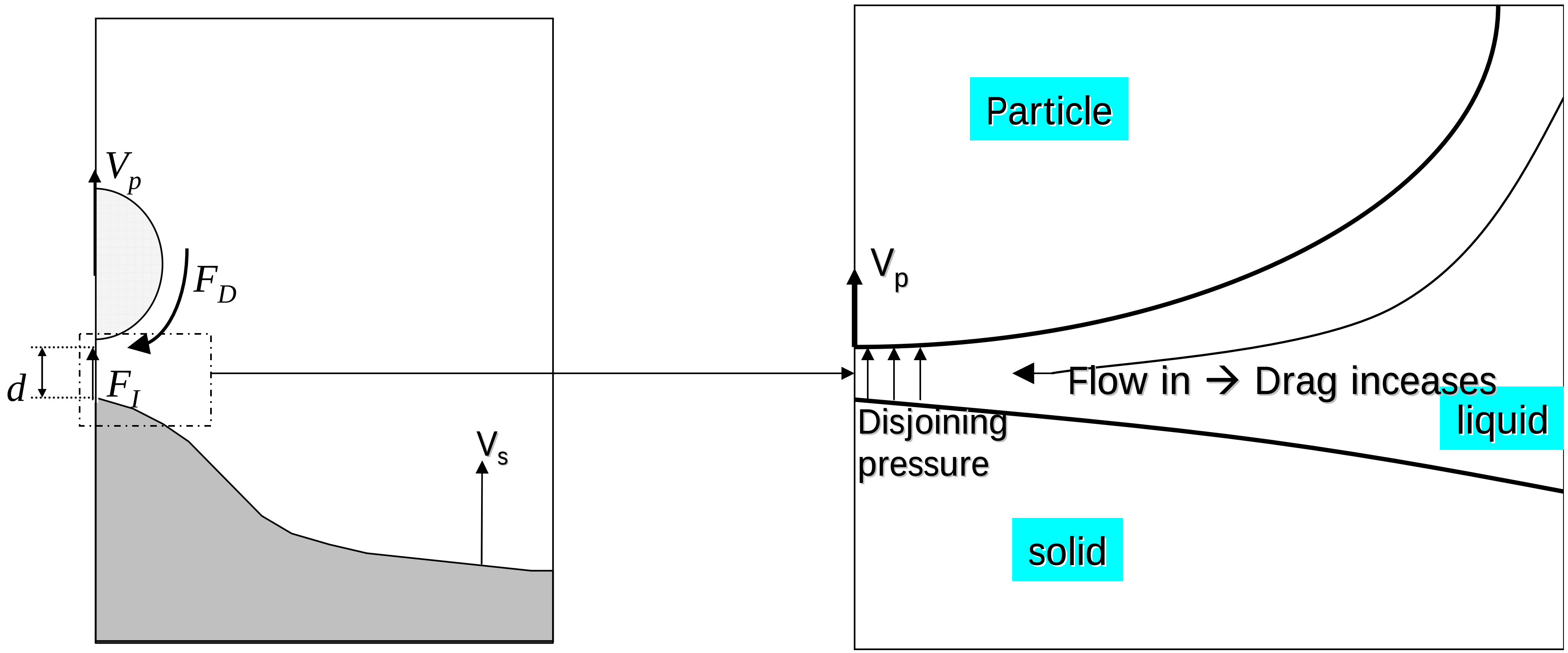
- Force balance on the particle

$$m_p \frac{dV_p}{dt} = F_I - F_D$$

- F_I is the repulsive interaction force
- F_D is an attractive drag force
- Balance determines whether the particle will be engulfed/pushed



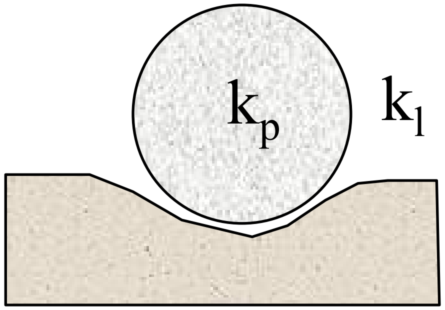
Fluid mechanics and thermal transport



- In addition, thermal conditions affect the critical velocity. Large scale effects (thermal conductivity differences between the particle and the solidification front), and small scale effects (premelting film).

The thermal conductivity issue

- k_p/k_l has a significant impact on whether a particle is pushed/engulfed

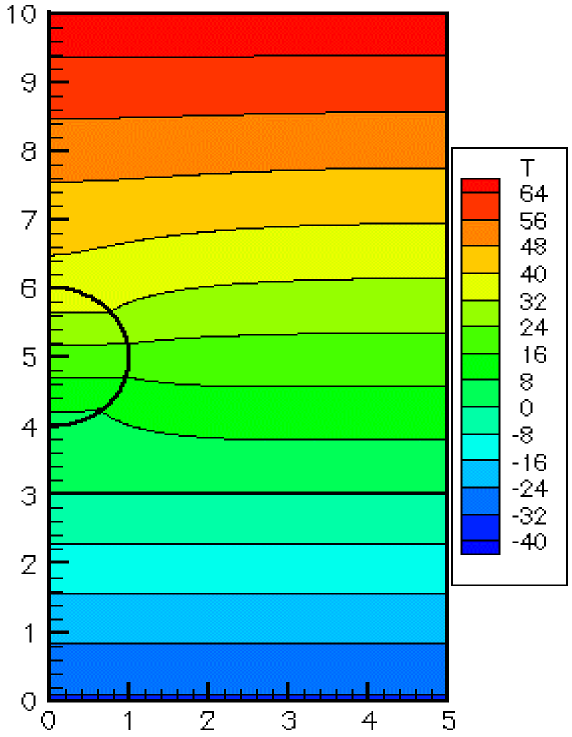


- In fact, experimental observations have shown that:
  - Engulfment 100% of the time for $k_p/k_l > 1.0$
  - Pushing for $k_p/k_l < 1.0$

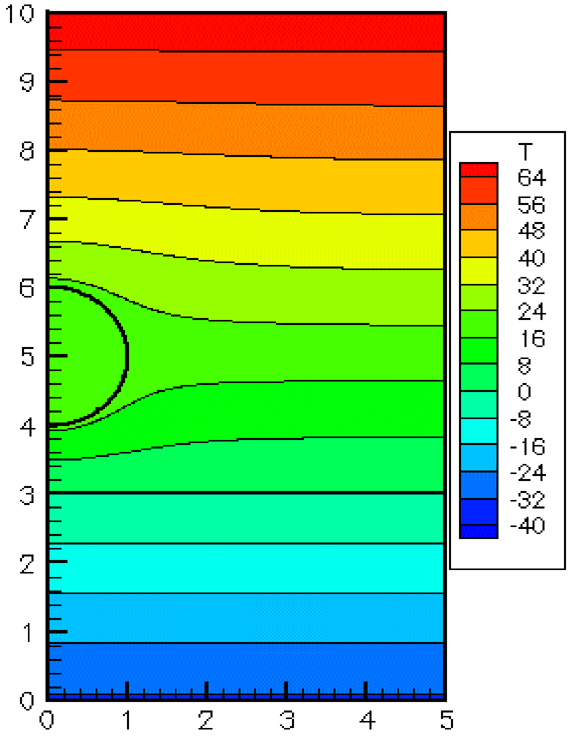
- Why does the k_p/k_l have such a significant impact?

How does the k_p/k_l influence the interface shape?

$k_p/k_l < 1.0$



$k_p/k_l > 1.0$



<u>Summary</u>: The thermal conductivity ratio, k_p/k_l, has a significant impact on whether a particle is pushed/engulfed → this is a micro-scale phenemenon (scale of the particle)

What about nano-scale phenomena?

Premelted films

$T < T_m$

Film thickness: $d = (-2\sigma^2 \frac{\Delta\gamma}{\rho_l \Delta H_f})^{1/3} t^{-1/3}$

Atomic radius: σ

Liquid density: ρ_l

Latent heat per molecule: ΔH_f

$$t = \frac{T_m - T_i}{T_m} \qquad \Delta\gamma = \gamma_{sp} - (\gamma_{lp} + \gamma_{ls})$$

Premelting film theory effect on interface temperature of a solidification front

$$T_i = T_m - \left(\frac{\lambda}{d}\right)^{\upsilon} T_m$$

T_i is the interface temperature
T_m is the melting temperature

ν= 3 for van der Waals
λ is an interaction length scale (nanometer scale)

Disjoining pressure theory

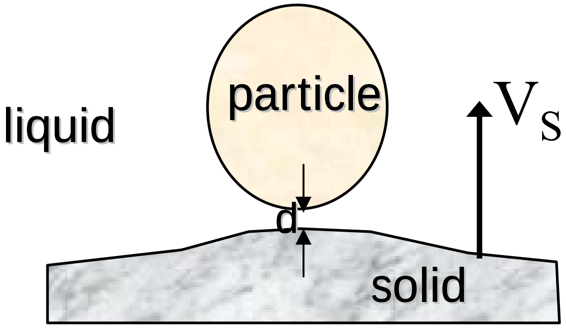
- Disjoining pressure ⟶ $$\Pi = \frac{A}{6\pi d^3}$$
  - Nano-scale force
  - Molecular in nature

A = Hamaker constant $\sim \Delta\gamma$

$\Delta\gamma = \gamma_{sp} - (\gamma_{lp} + \gamma_{ls})$ ⟶

$\Delta\gamma > 0$ → repulsive

$\Delta\gamma < 0$ → attractive

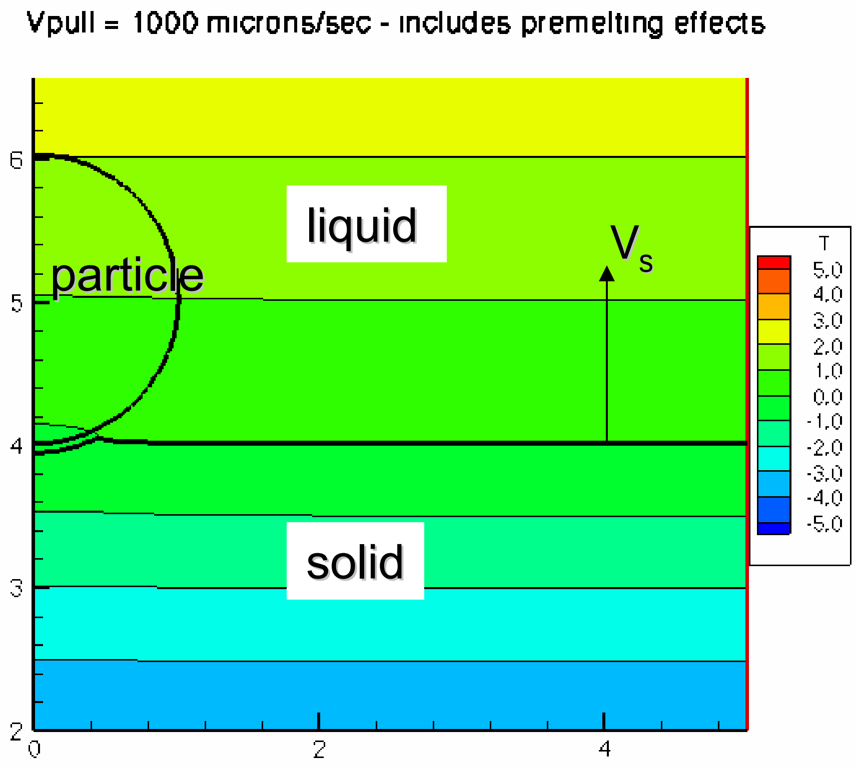


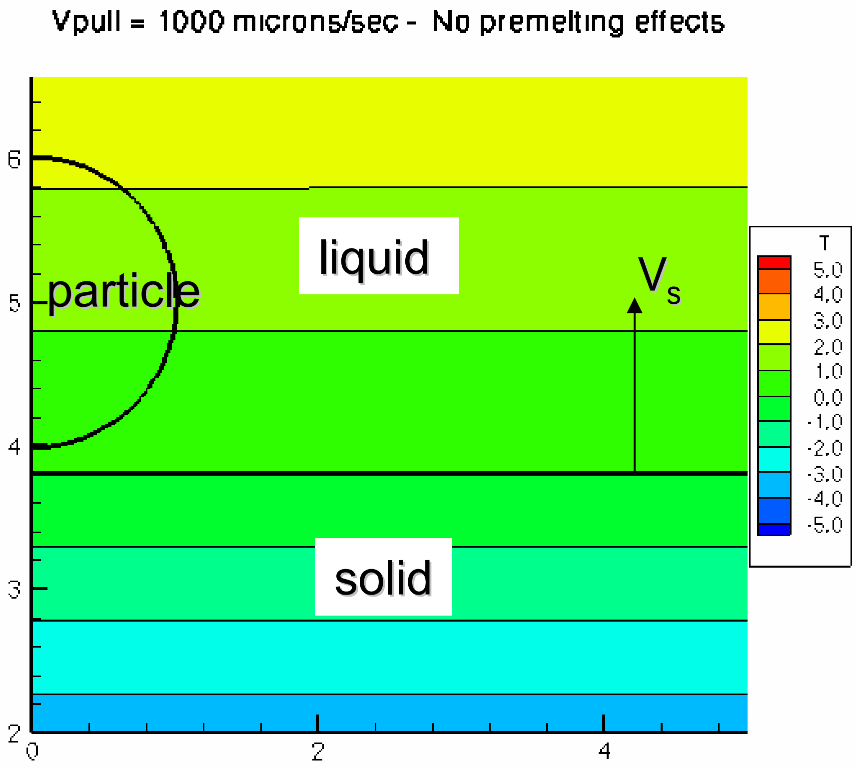
- Van der Waals?

Previous work on thermal effects of premelted layers on particle-solidification front dynamics

(Garvin and Udaykumar, Journal of Crystal Growth (2005))

Premelting film theory effect on interface temperature of a solidification front


Vpull = 1000 microns/sec - includes premelting effects

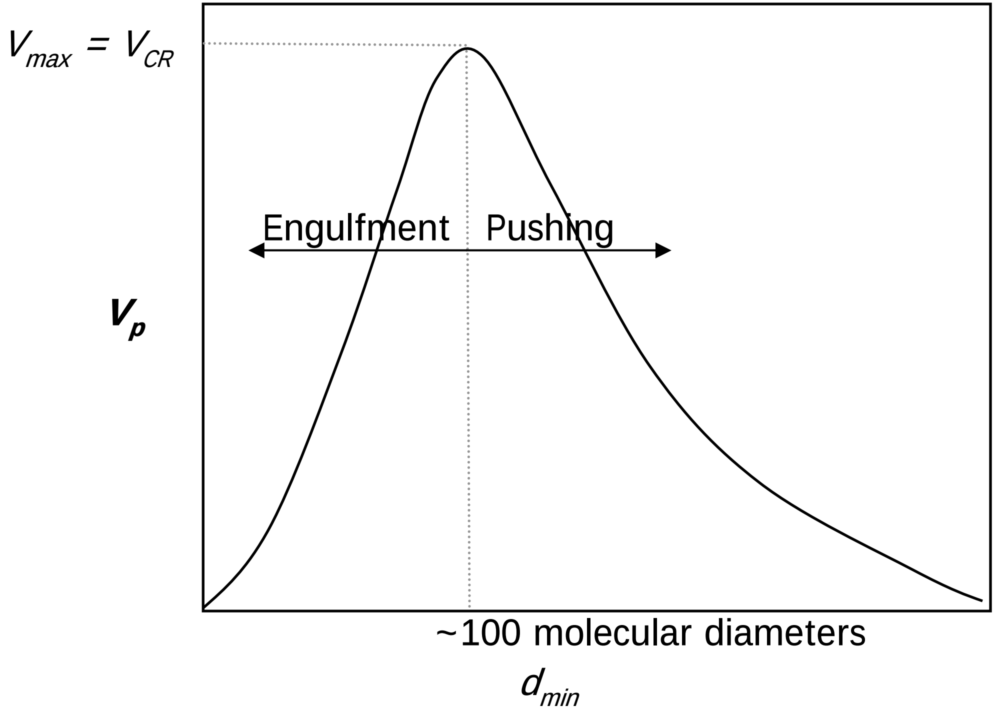

Vpull = 1000 microns/sec - No premelting effects

$$T_i = T_m - \left(\frac{\lambda}{d}\right)^{\nu} T_m$$

$$T_i = T_m$$

The premelting effect on V_{CR}

- 2 approaches when modeling
  1) Not to include premelting in the interaction
     - Requires setting a gap thickness cut-off value for engulfment (ad hoc)
  2) Including premelting (Rempel and Worster)
     - Linear stability analysis, steady-state and $k_p/k_l = 1.0$
     - No need for ad-hoc cut-off for gap thickness



Summary of physics

- k_p/k_l ratio greatly affects the critical velocity (micro-scale effect)
  - Alters the interface shape
    - $k_p/k_l < 1.0$, bump forms that promotes pushing
    - $k_p/k_l > 1.0$, trough forms that promotes engulfing (higher drag)

- Premelting film
  - Liquid layer wants to exist between the front and the particle
    - Also alters interface shape
    - If no premelting is assumed, gap thickness cut-off value is needed

The k_p/k_l effects act on a larger (microscale) whereas the premelting/disjoining pressure effects act on a “nano”-scale

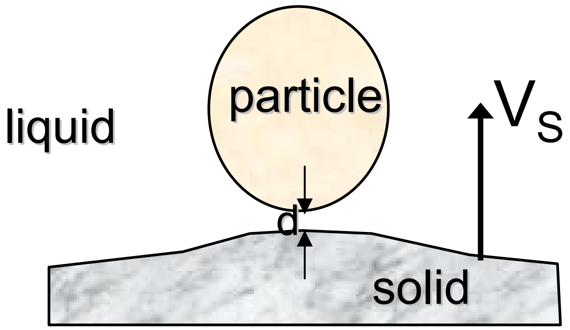
PROBLEM: How to model particle-solidification front interactions?

In the past …

– Theoretical research relied on…

1) All-simplified models for the forces acting on the particle
2) All-qualitative explanations/models based off of thermal property considerations
3) Most on steady-state analysis
4) Most- Do not assume a premelting layer in the gap
5) All-assumed stable (non-dendritic solidifications front)

ALL MODELS ATTEMPT TO FIND CRITICAL VELOCITY



OUR APPROACH…

Lubrication Model for the flow in the gap between the front and particle and NS for outer flow – match solutions (matched numerics)

Advantages

1. Capture dynamics (i.e. not a steady-state solution)

2. Premelting effects will be included

3. k_p/k_l effects will be captured from the governing equation

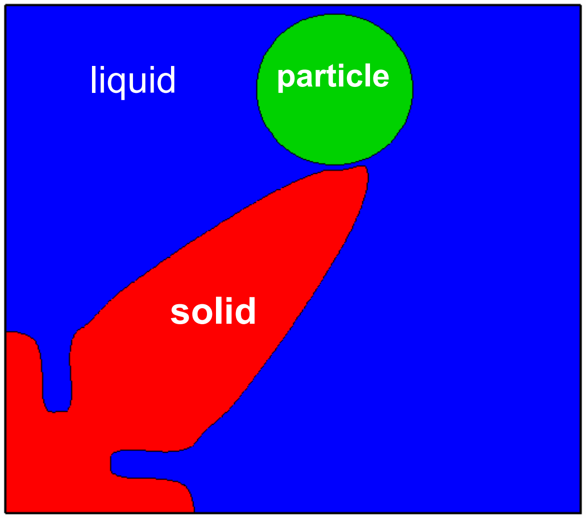
4. Do not have to rely on simple force models as the lubrication equation will contain a repulsive body force

5. Can be generalized for a variety of problems involving solid body interactions (including dendrite+particle)

Modeling of particle-front interactions

Main Ingredients:

1. Solidification front and the particle are tracked using a sharp-interface level-set method with transport variables solved via NS equations "outer region"
2. Solution in the gap in treated as a lubrication layer, so a different set of equations are needed "inner region"
3. The solution of the "inner" and "outer" regions are coupled through BCs. "matching region"



Outer transport equations

- Navier-Stokes Equations (with mass and energy conservation):

Continuity equation:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0$$

x-Momentum equation:

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = -\frac{1}{\rho}\frac{\partial p}{\partial x} + \frac{\mu}{\rho}\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)$$

y-Momentum equation:

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} = -\frac{1}{\rho}\frac{\partial p}{\partial y} + \frac{\mu}{\rho}\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right)$$

Energy equation:

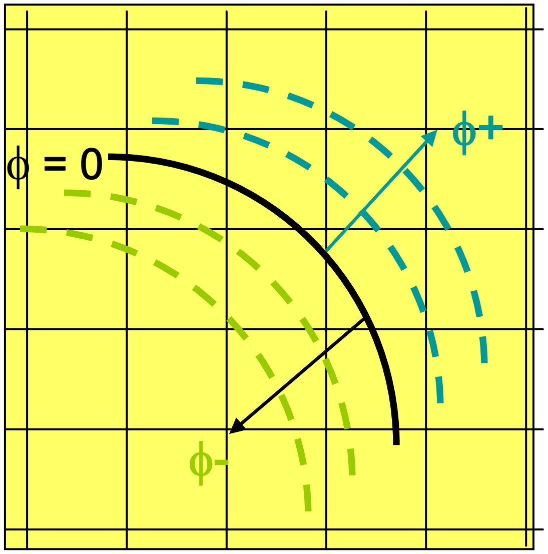
$$\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial y} = \alpha_{s/l/p}\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right)$$

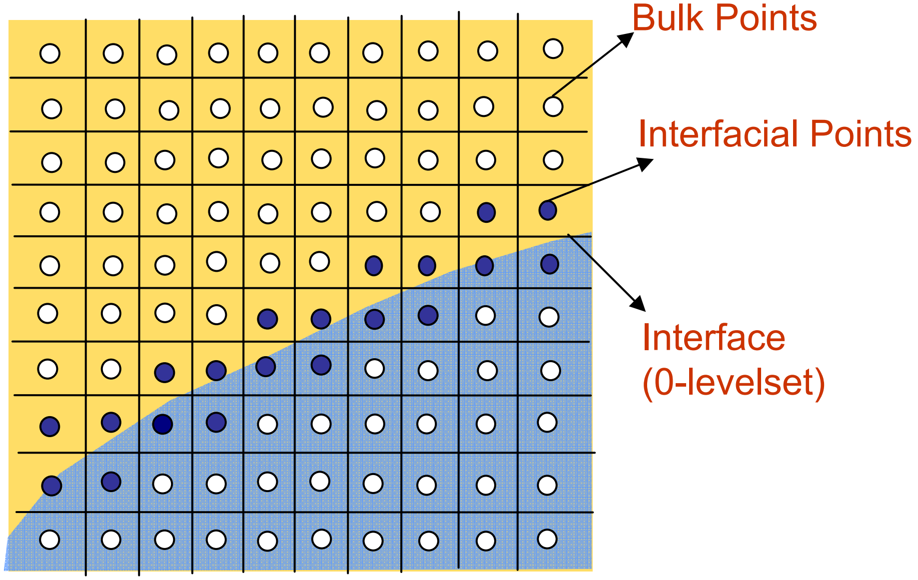
Interface conditions:

$$\rho H_{sl} V_N = k_s \left.\frac{\partial T}{\partial n}\right|_s - k_l \left.\frac{\partial T}{\partial n}\right|_l$$

Level-Set Method

Level-set function (ϕ) - Signed normal distance from the interface





$$\phi_t + \vec{V} . \vec{\nabla} \phi = 0$$

Level-set Advection

$$\vec{N} = \vec{\nabla} \phi \Big/ \left| \vec{\nabla} \phi \right|$$

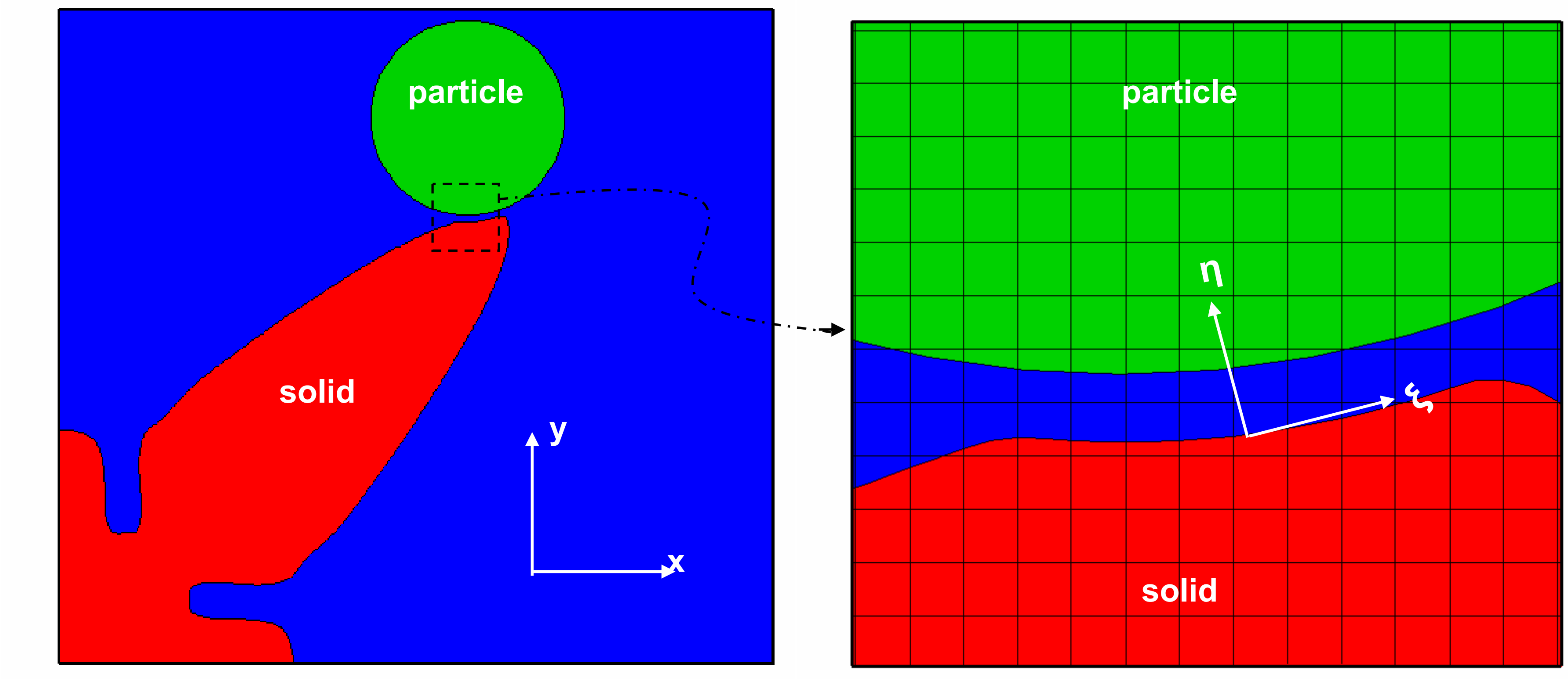
Normal

$$\kappa = -\vec{\nabla} . \vec{N}$$

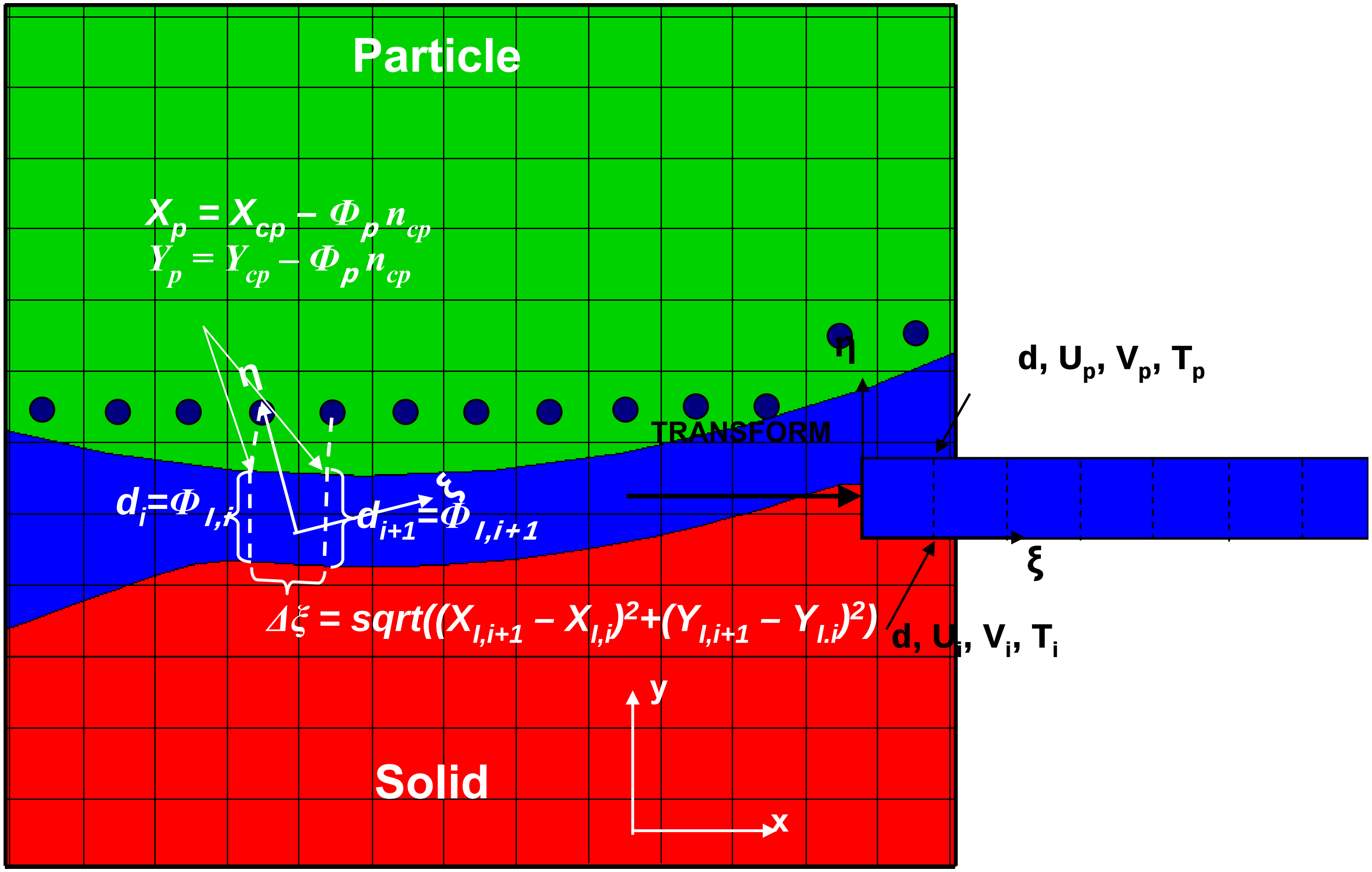
Curvature

Using a Lubrication Model for “inner” region

- Lubrication Model
  - One direction of the fluid flow and the heat flow is assumed to have negligible effects compared to other directions
  - The need for a mesh in one direction is eliminated
    - Interaction in the gap (disjoining pressure included) can be accounted for in lubrication model



Using a Lubrication Model for “inner” region



Transformed NS equations from x,y → ξ,η

Continuity:

$$\frac{\partial U}{\partial \xi} + \frac{\partial V}{\partial \eta} = 0$$

u-momentum (v-momentum and Energy equation are very similar):

$$\frac{\partial (J\rho u)}{\partial t} + \frac{\partial (\rho U u)}{\partial \xi} + \frac{\partial (\rho V u)}{\partial \eta} = -\left\{ \frac{\partial y}{\partial \eta}\frac{\partial p}{\partial \xi} - \frac{\partial y}{\partial \xi}\frac{\partial p}{\partial \eta} \right\} + \frac{\partial}{\partial \xi}\left[\frac{\mu}{J}\left(q_1 \frac{\partial u}{\partial \xi} - q_2 \frac{\partial u}{\partial \eta} \right) \right] + \frac{\partial}{\partial \eta}\left[\frac{\mu}{J}\left(q_3 \frac{\partial u}{\partial \eta} - q_2 \frac{\partial u}{\partial \xi} \right) \right] - \underbrace{\left\{ \frac{\partial y}{\partial \eta}\frac{\partial \Pi}{\partial \xi} - \frac{\partial y}{\partial \xi}\frac{\partial \Pi}{\partial \eta} \right\}}_{\text{Disjoining Pressure terms treated as body force}}$$

Where: u,v → x,y velocities;
U,V → ξ, η velocities,

Orthogonal coordinates (q_2=0) and do scaling analysis

Scaling: $\xi^* = \frac{\xi}{L}$ $\quad$ $\eta^* = \frac{\eta}{d}$

By assuming small curvatures in the interfaces and using the fact that:

$$U = uy_\eta - vx_\eta \qquad V = vx_\eta - uy_\xi$$

To get:

Mass: $$\frac{\partial U^*}{\partial \xi^*} + \frac{\partial V^*}{\partial \eta^*} = 0$$

U-mom: $$-\left(\frac{\left(J^*\right)^3}{J^*_{NO} q_3^*}\right)\left(\frac{\partial p^*}{\partial \xi^*} + \frac{\partial \Pi^*}{\partial \xi^*}\right) + \frac{\partial^2 U^*}{\partial \eta^{*2}} = 0$$

V-mom: $$\left(\frac{\partial p^*}{\partial \eta^*} + \frac{\partial \Pi^*}{\partial \eta^*}\right) = 0$$

Energy: $$\frac{\partial^2 T^*}{\partial \eta^{*2}} = 0$$

Notice that p^* and Π^* only depend on ξ^*

Pressure Equation in the gap

$$-\left(\frac{(J)^3}{J_{NO}q_3}\right)\left[\left(\frac{\partial^2 p}{\partial\xi^2}+\frac{\partial^2\Pi}{\partial\xi^2}\right)\frac{d^3}{12}+\left(\frac{\partial p}{\partial\xi}+\frac{\partial\Pi}{\partial\xi}\right)\frac{\partial d}{\partial\xi}\left(\frac{d^2}{4}\right)\right]+\frac{1}{2}\left(d\,\frac{\partial(U_p-U_i)}{\partial\xi}+(U_p-U_i)d^2\frac{\partial}{\partial\xi}\left(\frac{1}{d}\right)\right)+V_p-V_i=0$$

BCs: At $\xi=0$, $p=p_{outer,0}$
At $\xi=L$, $p=p_{outer,L}$

Temperature Equation: $T=\left(\frac{T_p-T_i}{d}\right)\eta+T_i$

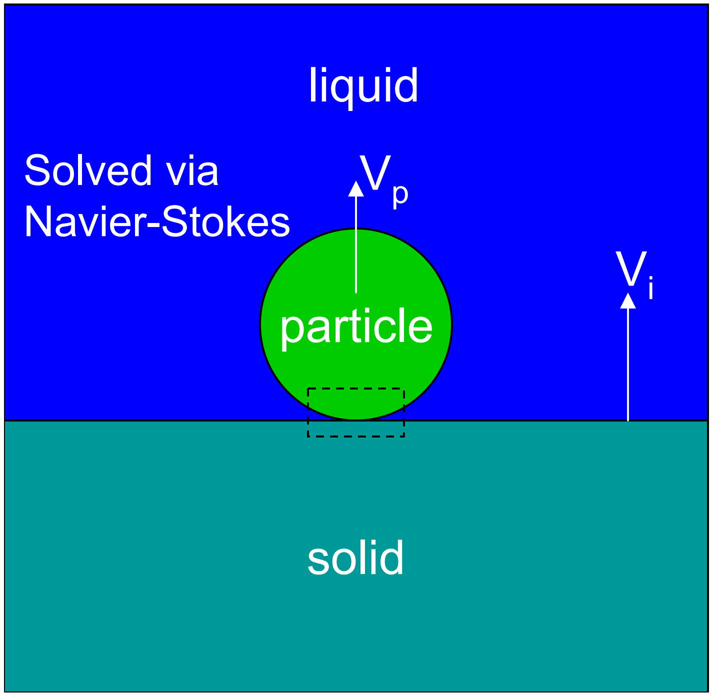
Coupling the outer flow equations to the inner lubrication equations

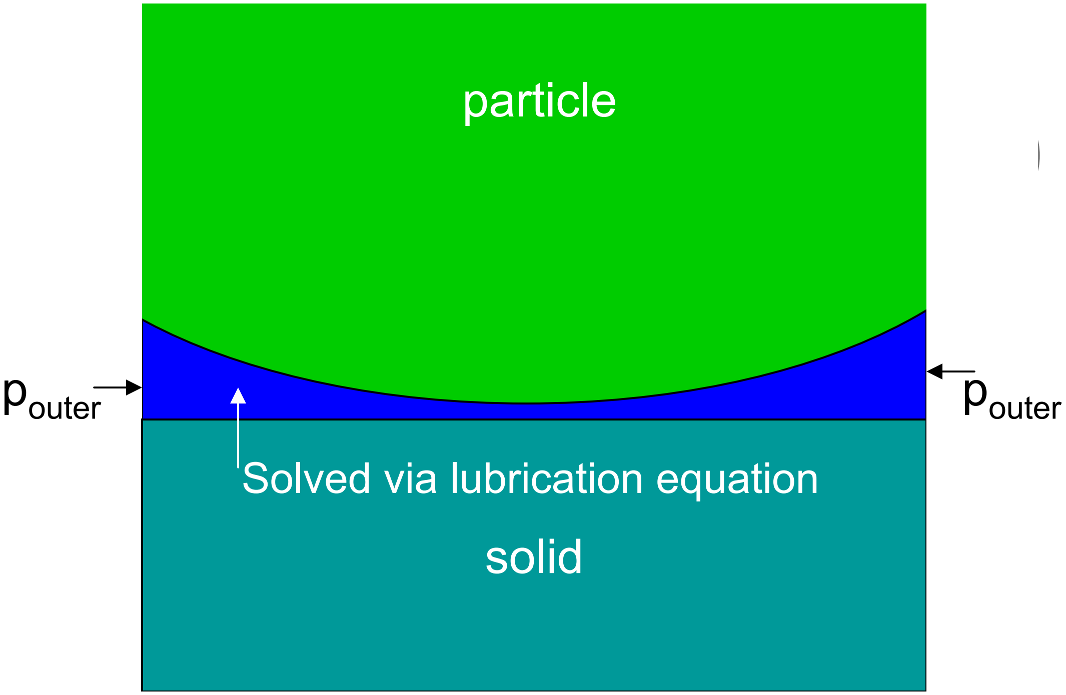
How are the Boundary conditions applied to the lubrication model?

BCs: At $\xi=0$, $p=p_{outer}$

At $\xi=L$, $p=p_{outer}$

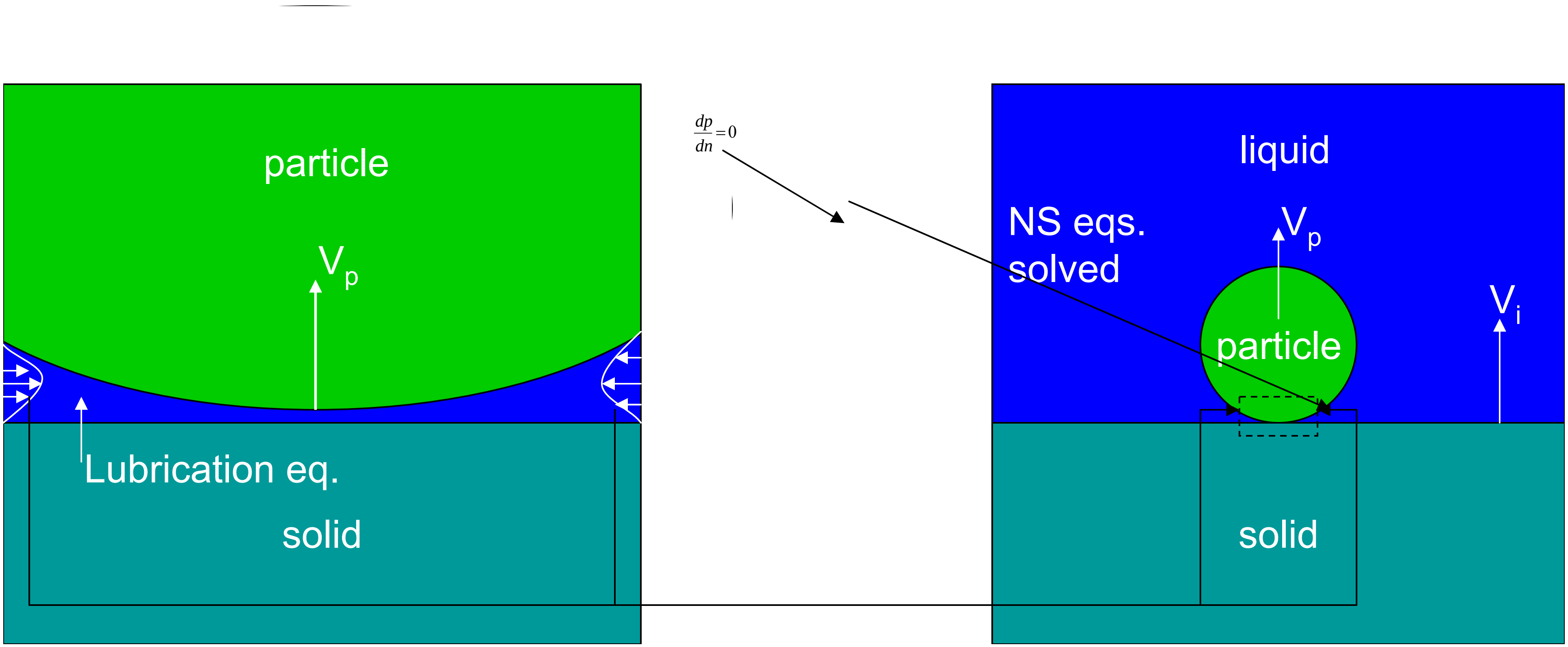
Edge of the lubrication layer is 8 mesh pts. → enough resolution for outer flow





How are the Boundary conditions applied to the outer flow (solved via NS)?

BCs: at the edges of lubrication layer, find a parabolic velocity profile that satisfies mass conservation (treated as outlets)



Forces acting on the bodies

The forces acting on the bodies can now be obtained from the outside flow and the inner lubrication flow, so:

$$\sum \vec{F} = \vec{F}_{INNER} + \vec{F}_{OUTER}$$

$$\vec{F}_{INNER} = -\int_{A} p_{INNER}\, d\vec{S}$$

$$\vec{F}_{OUTER} = -\int_{A} p_{OUTER}\, d\vec{S}$$

The temperature of the interfaces?

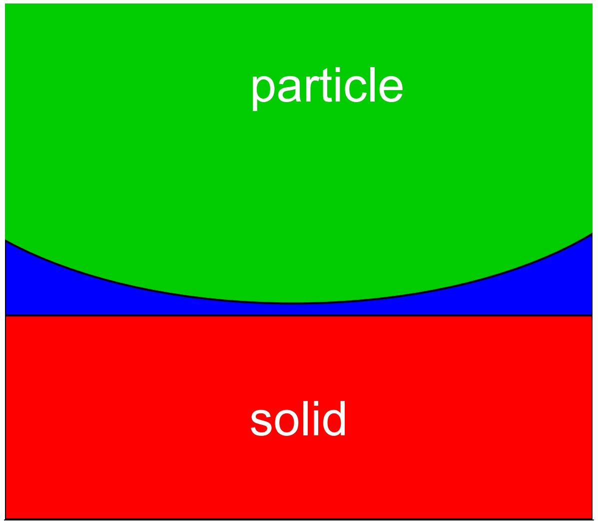
Temperature of the solidification front is found via:

$$T_i = T_m - \left(\frac{\lambda}{d}\right)^{\upsilon} T_m \longrightarrow \text{premelting}$$

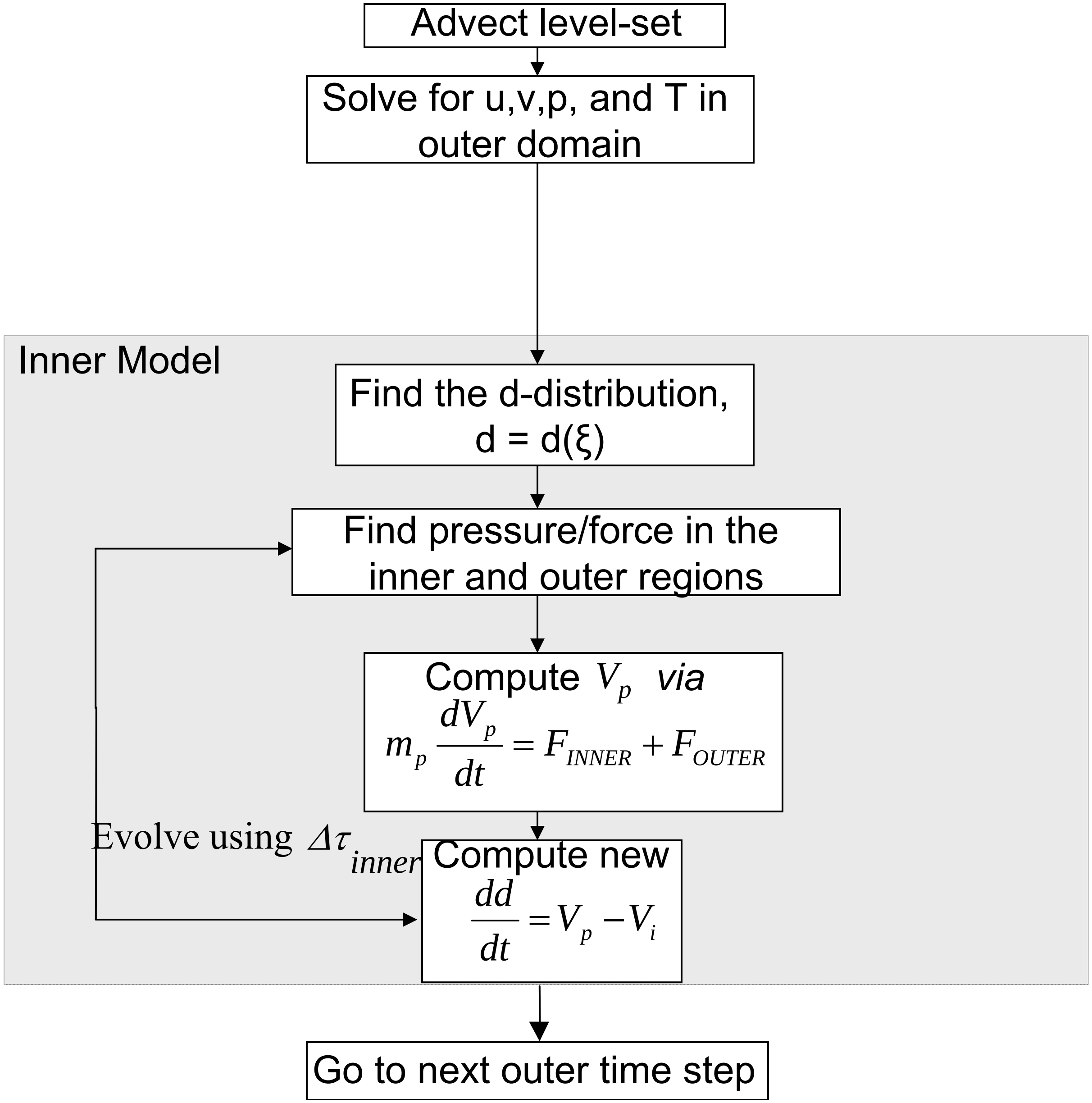
$$T_i = T_m \longrightarrow \text{No premelting}$$

The d-distribution is found from the level set information
The particle interface temperature is found from:

$$T_p = \left(\frac{q''}{k_l}\right) d + T_i$$



Flowchart of calculation



Advect level-set

Solve for u,v,p, and T in outer domain

Inner Model

Find the d-distribution, d = d(ξ)

Find pressure/force in the inner and outer regions

Compute V_p *via*

$$m_p \frac{dV_p}{dt} = F_{INNER} + F_{OUTER}$$

Evolve using $\Delta\tau_{inner}$

Compute new

$$\frac{dd}{dt} = V_p - V_i$$

Go to next outer time step

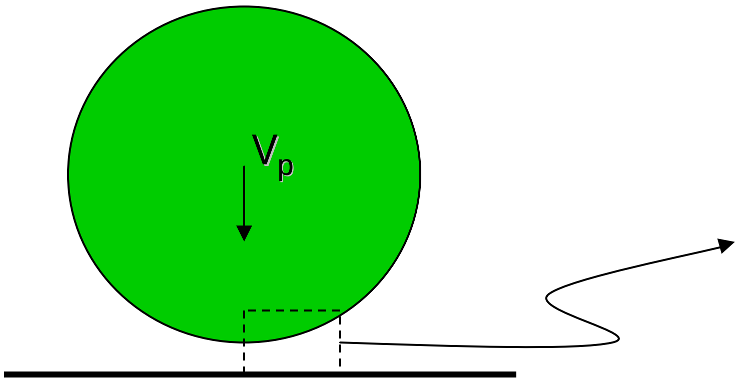
Results for particle+stable (non-dendritic) solidification front

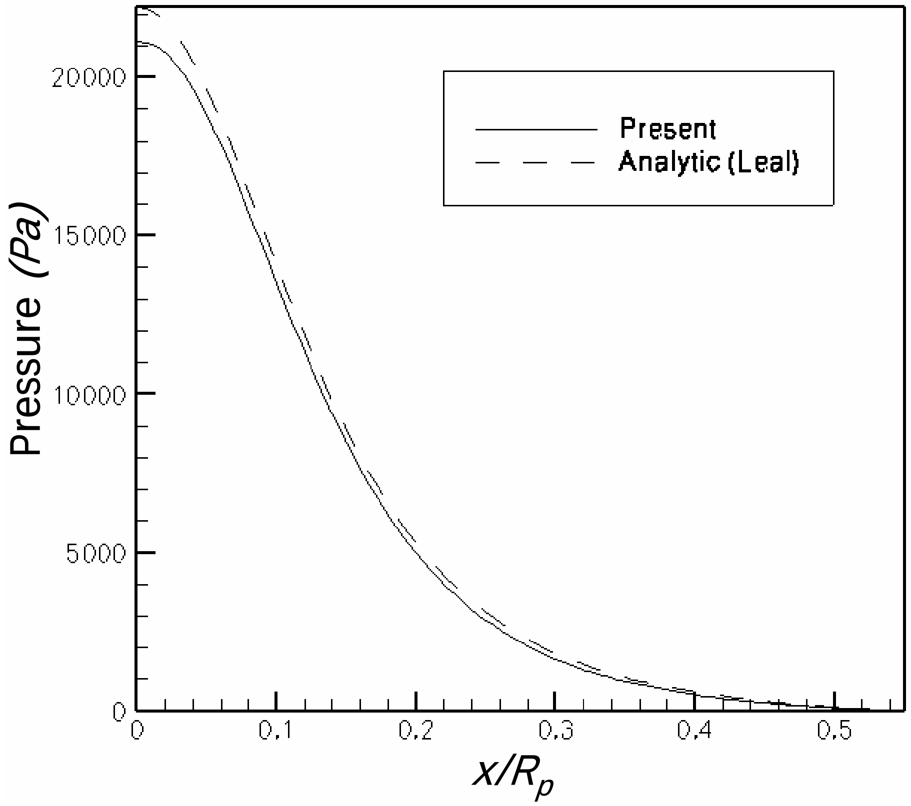
Validation of coupled model

-Compare model solution to an analytic solution for a simplified case

  -Particle approaching flat stationary interface (no disjoining pressure)[1]

-d/R_p = 0.02, Particle velocity = 500 microns/sec, R_p = 1 micron





1. Gary L. Leal, Laminar flow and convective transport processes : scaling principles and asymptotic analysis (1992).

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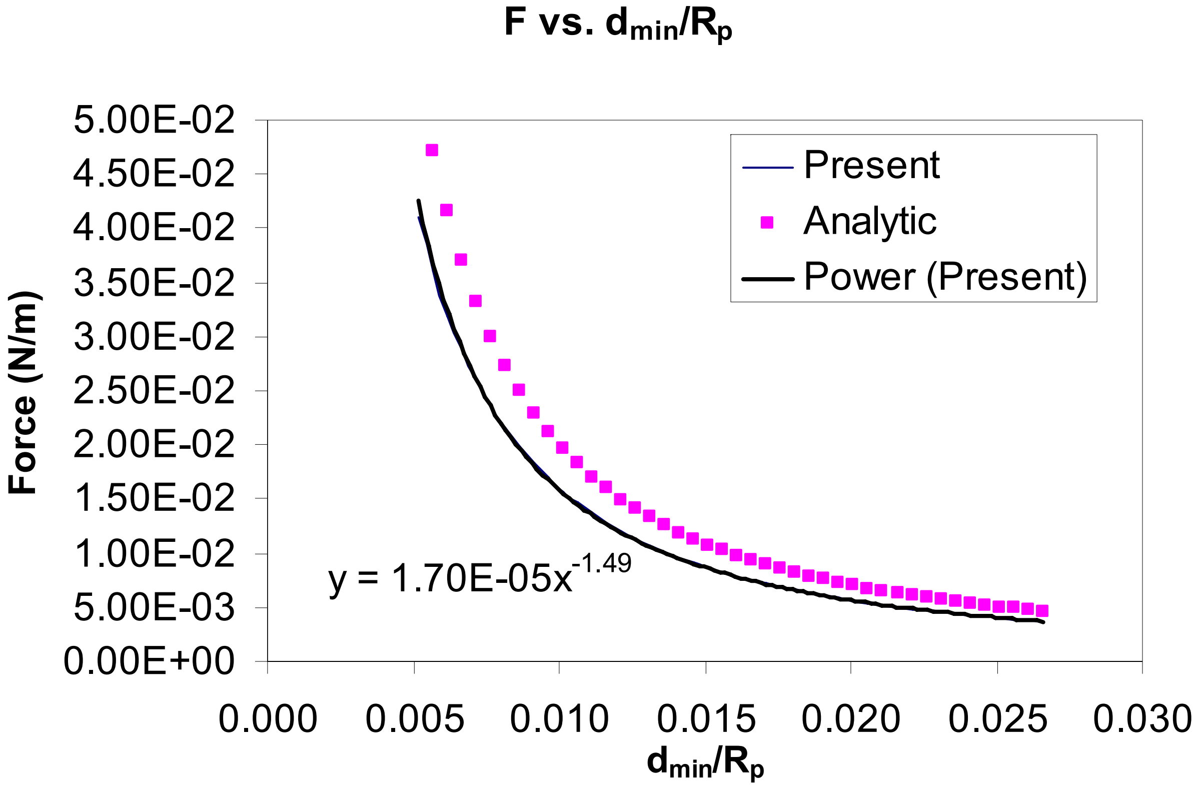
  -Particle approaching flat stationary interface (no disjoining pressure)[1]

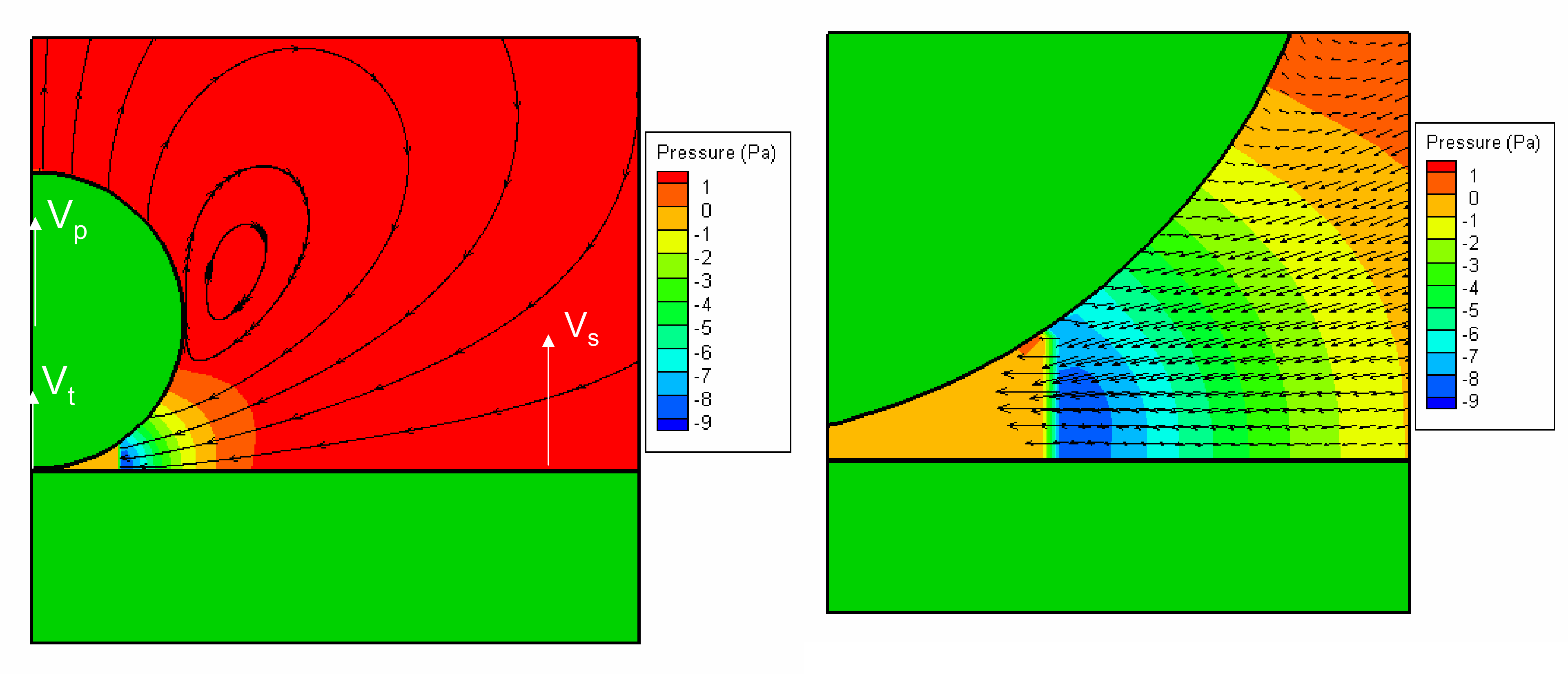
-Particle velocity = 500 microns/sec, R_p = 1 micron



1. Gary L. Leal, Laminar flow and convective transport processes : scaling principles and asymptotic analysis (1992).

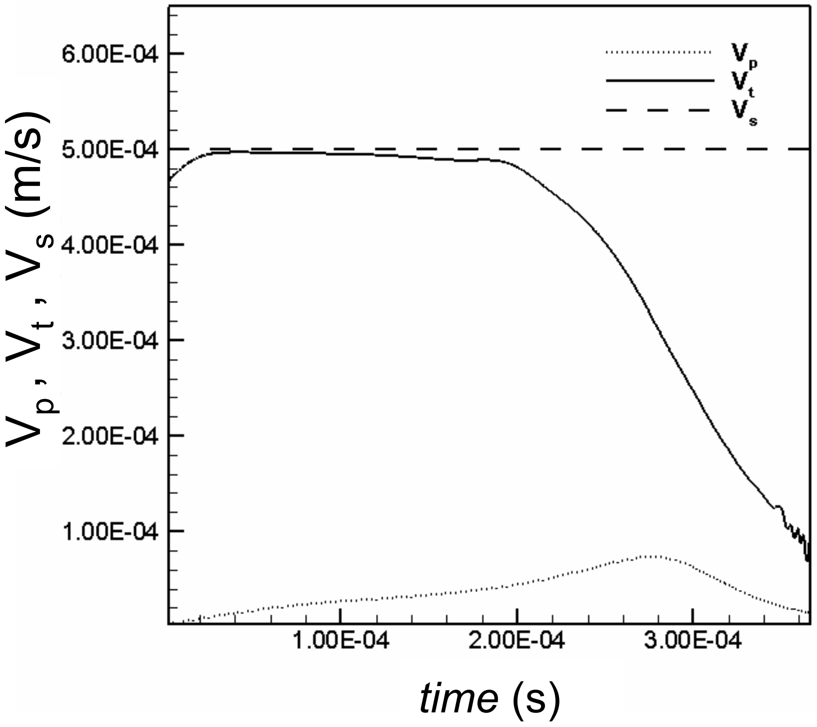
Planar Solidification front + particle

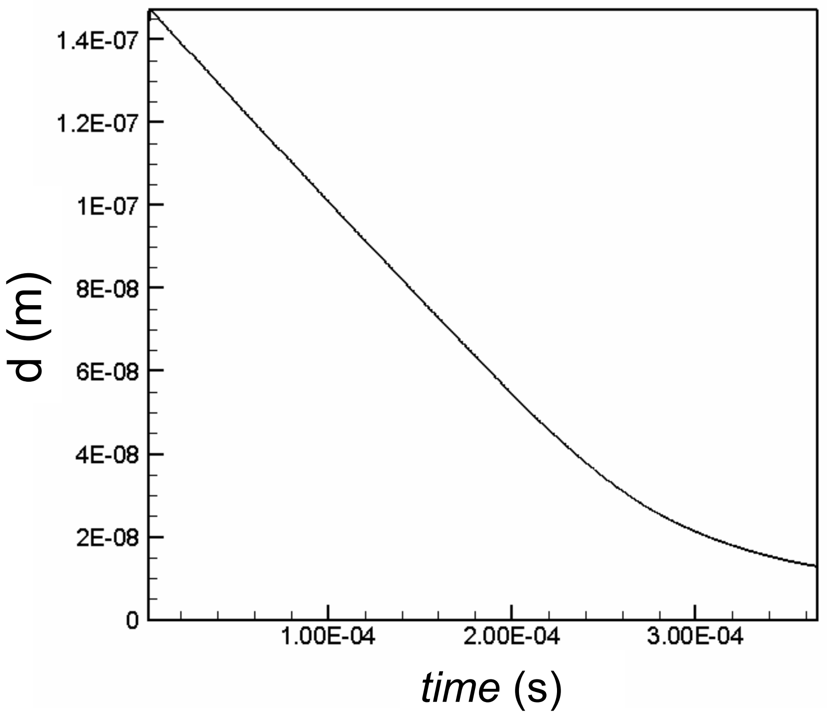
Solidification velocity = 500 microns/sec, R_p = 1 micron, Hamaker = -8E-19 J, k_p/k_l = 1.0 (planar), no premelting



Velocity vs. t and d vs. t plots – premelting

Solidification velocity = 500 microns/sec, R_p = 1 micron, Hamaker = -8E-19 J,
k_p/k_l = 1.0 (planar), premelting

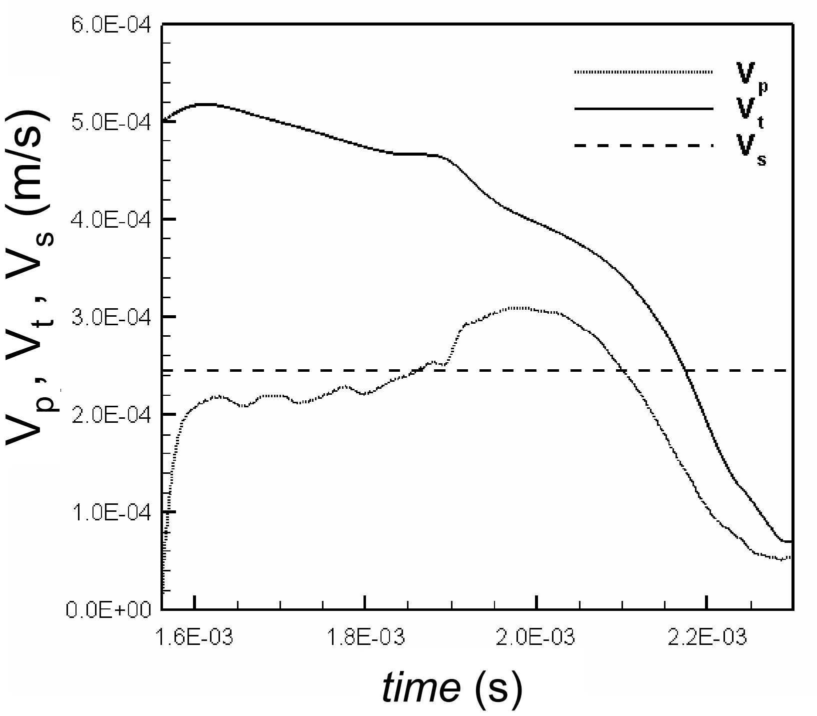


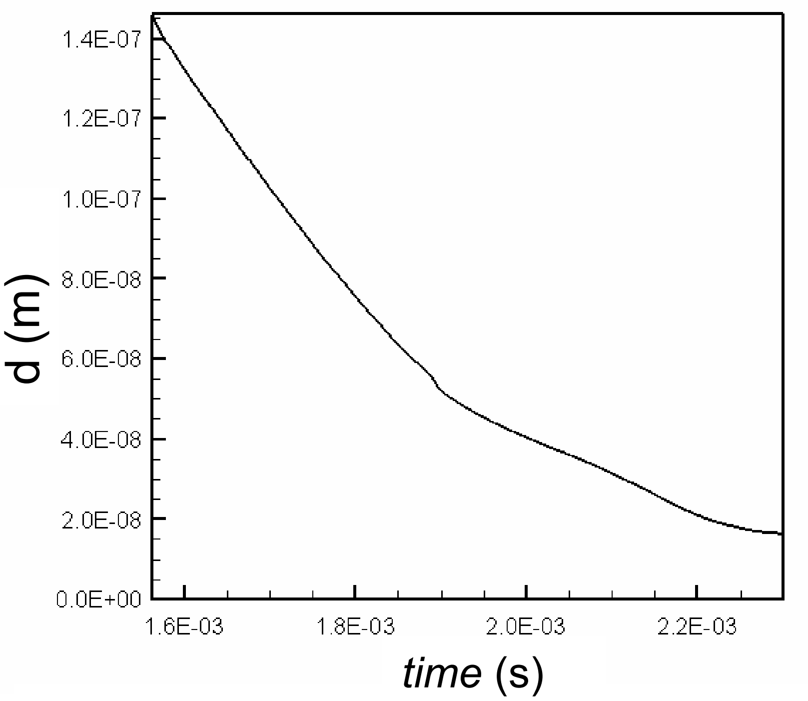


$k_p/k_l \geq 1.0$ ALWAYS ENGULFS!

What about $k_p/k_l < 1.0$

Solidification velocity = 245 microns/sec, R_p = 1 micron, Hamaker = -8E-19 J, k_p/k_l = 0.01 , premelting

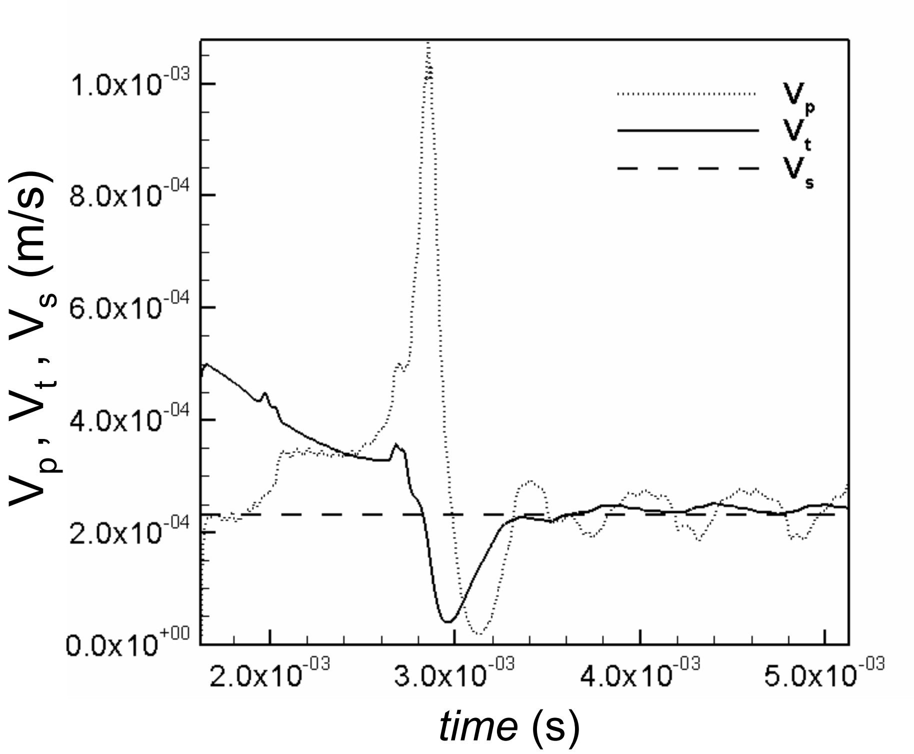


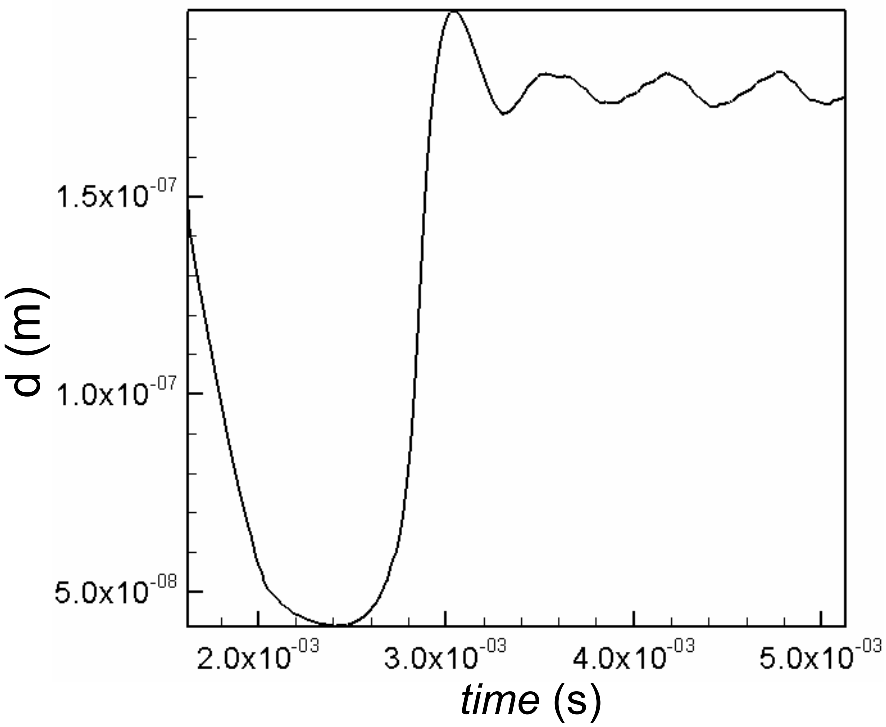


This one is engulfed!

What about $k_p/k_l < 1.0$

Solidification velocity = 230 microns/sec, R_p = 1 micron, Hamaker = -8E-19 J,
k_p /k_l = 0.01 , premelting

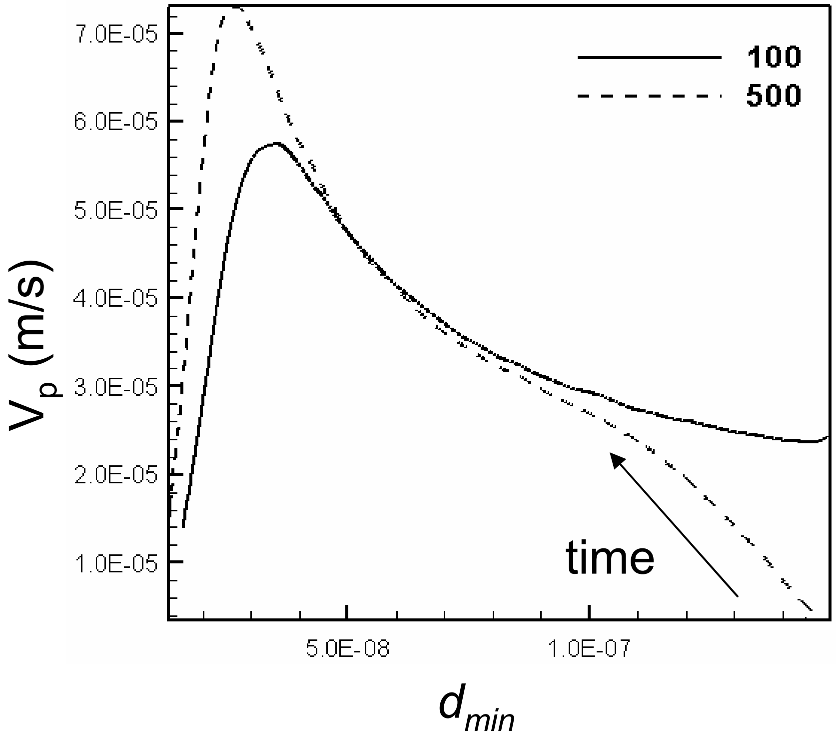




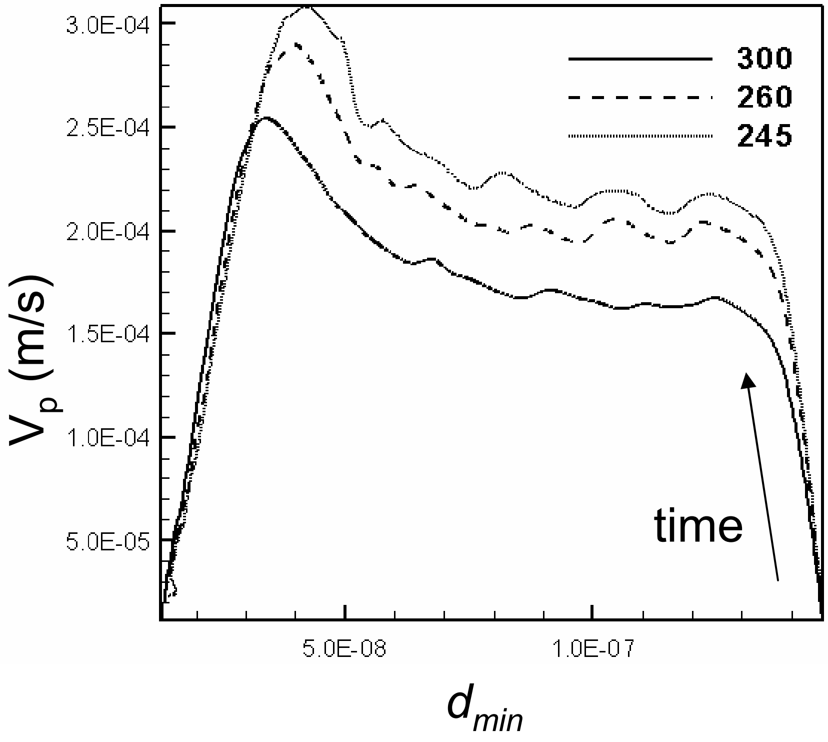
This one is Pushed!

Phase-Space Plots -- engulfment

$k_p/k_l = 1.0$



$k_p/k_l < 1.0$

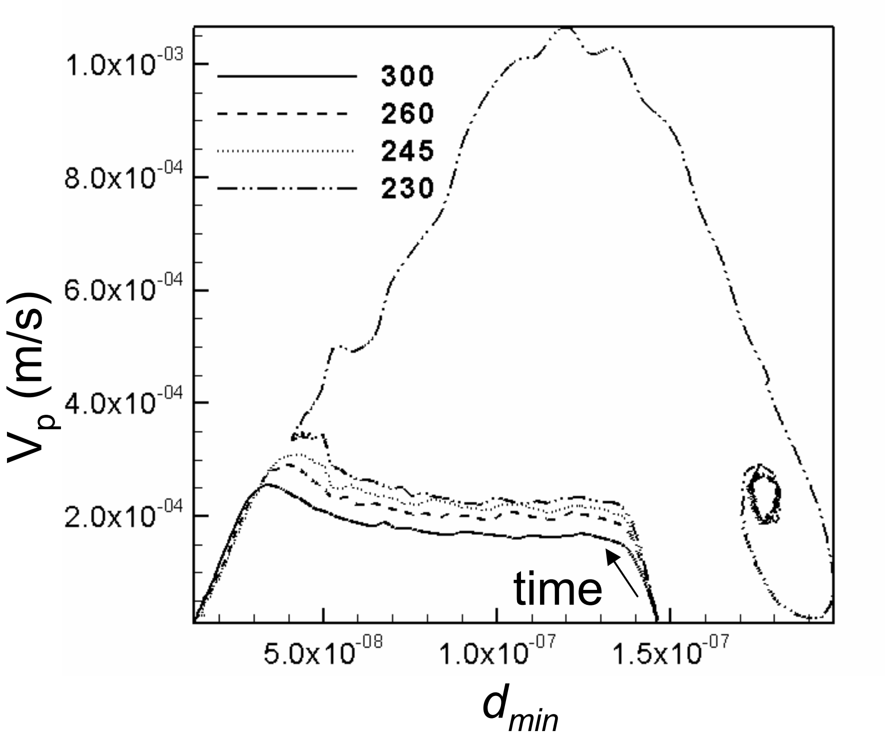


NOTE:

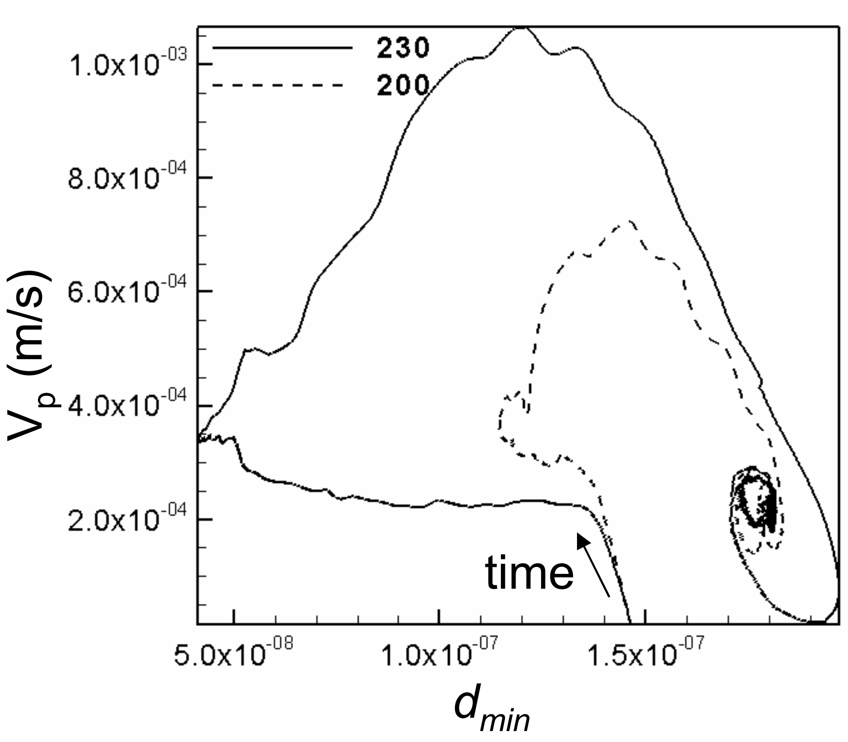
- Similarity to Rempel and Worster – steady-state
- $k_p/k_l = 1.0$ → Rempel and Woster claim pushing at certain values, current claim is always engulfment

Phase-Space Plots – engulfment/pushing

$k_p/k_l < 1.0$



$k_p/k_l < 1.0$



- 2 “attractors” in phase-space – engulfment/pushing
- Slightest change causes drastically different path to different region
- Reason: Interface never gets a chance to “bend”

Conclusions of results section:

1) For $k_p/k_l \geq 1$, engulfment always occurs

2) For $k_p/k_l < 1$, the critical velocity can be found from dynamical considerations and occurs the moment the solidification front velocity is such that the particle "outruns" the tip velocity

Main Contributions:

1. Developed a multiscale numerical approach to solve particle-solidification front problems in a general manner
2. Model captures essential physics that past research has neglected
3. First to look at the physics from a nonlinear dynamics point-of-view (i.e. phase-space point of view)
4. Model can be generalized to solve a variety of problems involving interacting interfaces

Overall Conclusions

A. Multiscale method was developed

1. Capturing the interaction dynamics between two arbitrary solid objects
2. Coupled two distinct regions (“inner” and “outer”) using a ‘matched numerics approach’

B. Application of interest

1. Particle-solidification front interactions
    a. Engulfment occurs for $k_p/k_l \geq 1$.
    b. For $k_p/k_l < 1$, the critical velocity is found using dynamical considerations
    c. No assumptions are made as to the force equations or the way in which the critical velocity is obtained (i.e. no cut-off gap thickness value), etc…