COMSOL model for the Capillary Breakup Extensional Electrorheometry (CaBEER) applied to functional inks

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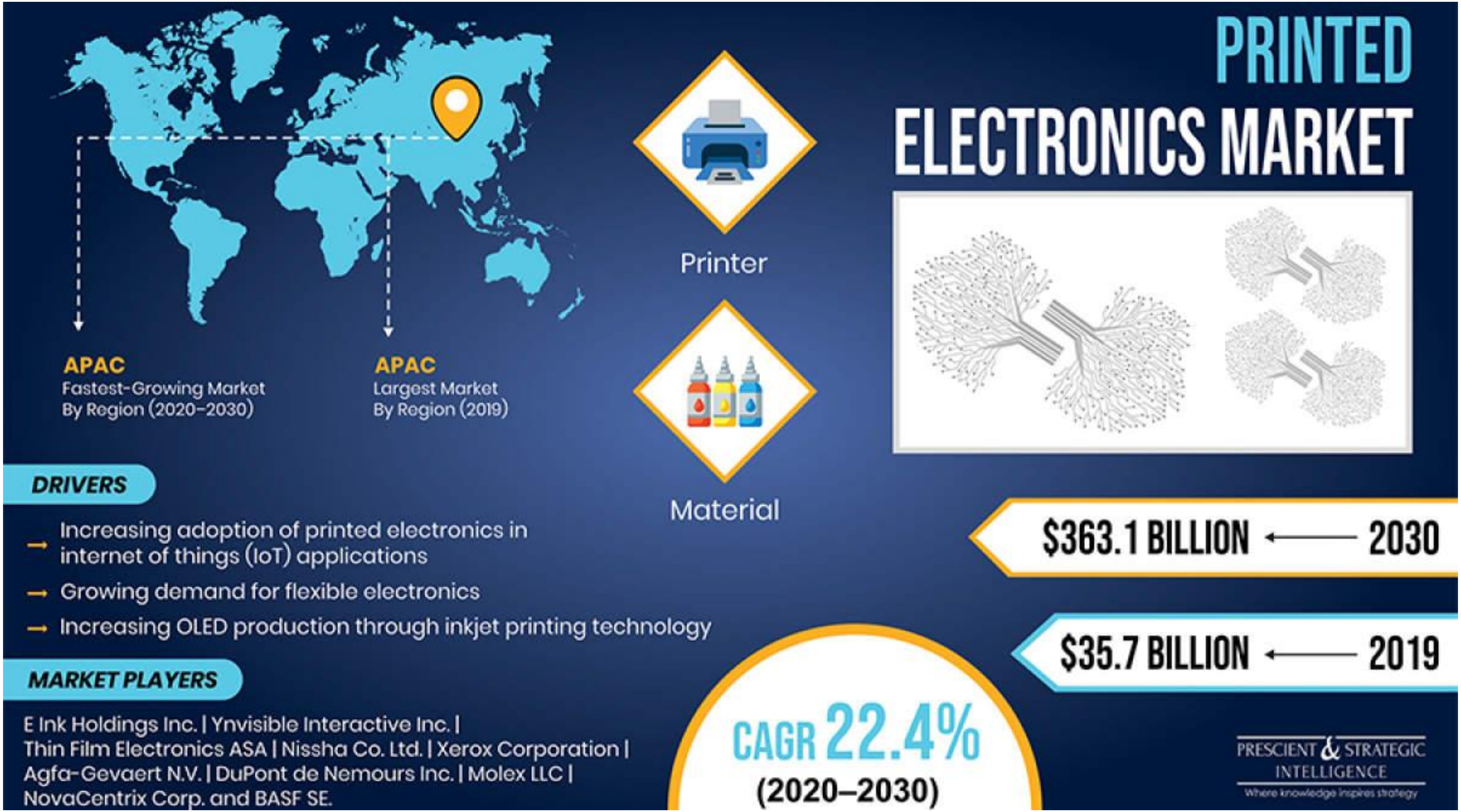
Supervisor: Emilio Ruiz Reina

25 de Junio de 2021

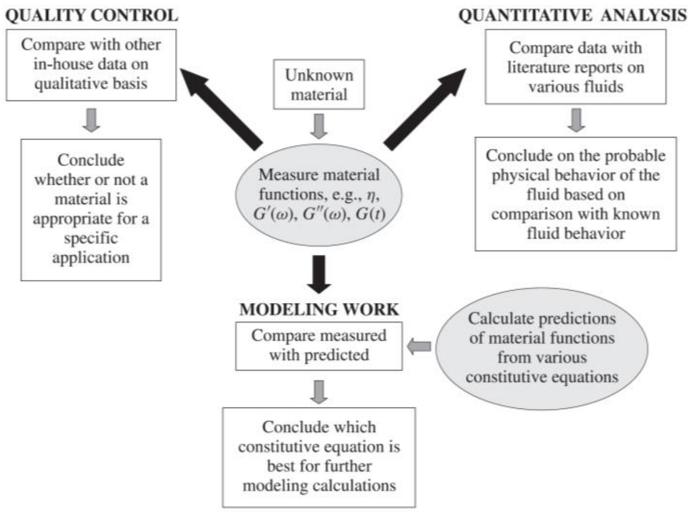
Master's Degree in Numerical Simulation in Science and Engineering with COMSOL Multiphysics (MUCOM)

Content



PRINTED
ELECTRONICS MARKET
APAC
Fastest-Growing Market
By Region (2020-2030)
APAC
Largest Market
By Region (2019)
Printer
Material
DRIVERS
Increasing adoption of printed electronics in internet of things (IoT) applications
Growing demand for flexible electronics
Increasing OLED production through inkjet printing technology
MARKET PLAYERS
E Ink Holdings Inc. | Ynvisible Interactive Inc. |
Thin Film Electronics ASA | Nissha Co. Ltd. | Xerox Corporation |
Agfa-Gevaert N.V. | DuPont de Nemours Inc. | Molex LLC |
NovaCentrix Corp. and BASF SE.
$363.1 BILLION 2030
$35.7 BILLION 2019
CAGR 22.4%
(2020–2030)
PRESCIENT & STRATEGIC
INTELLIGENCE
Where knowledge inspires strategy

Organic Photovoltaic
Consumer and first off-grid applications
Off-grid power, building integration
Grid-connected power generation
Flexible Display
Price labels, e-readers
High resolution colour e-readers, e-posters
Electronic wallpaper, rollable OLED TVs
OLED / EL Lighting
Small lamps, design and decorative applications
Light tiles, technical and architectural lighting
Flexible lighting elements
Printed RFID
Brand protection, e-ticketing
Logistics and automation
Item level tagging, EPC, identification
Printed Memory
Brand protection, identification, games
High end brand protection, advanced games
Electronics, multimedia
Organic Sensor
Photodiode, temperature, pressure, chemical
Potentiometric sensor array
Intelligent sensor, embedded systems
Flexible Battery
Low capacity, discontinuous use
Higher capacity, continuous use
Direct integration into packages, systems
Smart Objects
Greeting cards, animated logos
Intelligent tickets, initial smart packaging
Complex smart packaging
Smart Textiles
Clothing integrated keypads, sensors, light effects
Clothing integrated displays, photovoltaics
Fuel cells, fiber integrated sensors
© OE-A 2009
Today, Short term
Medium term
Long term

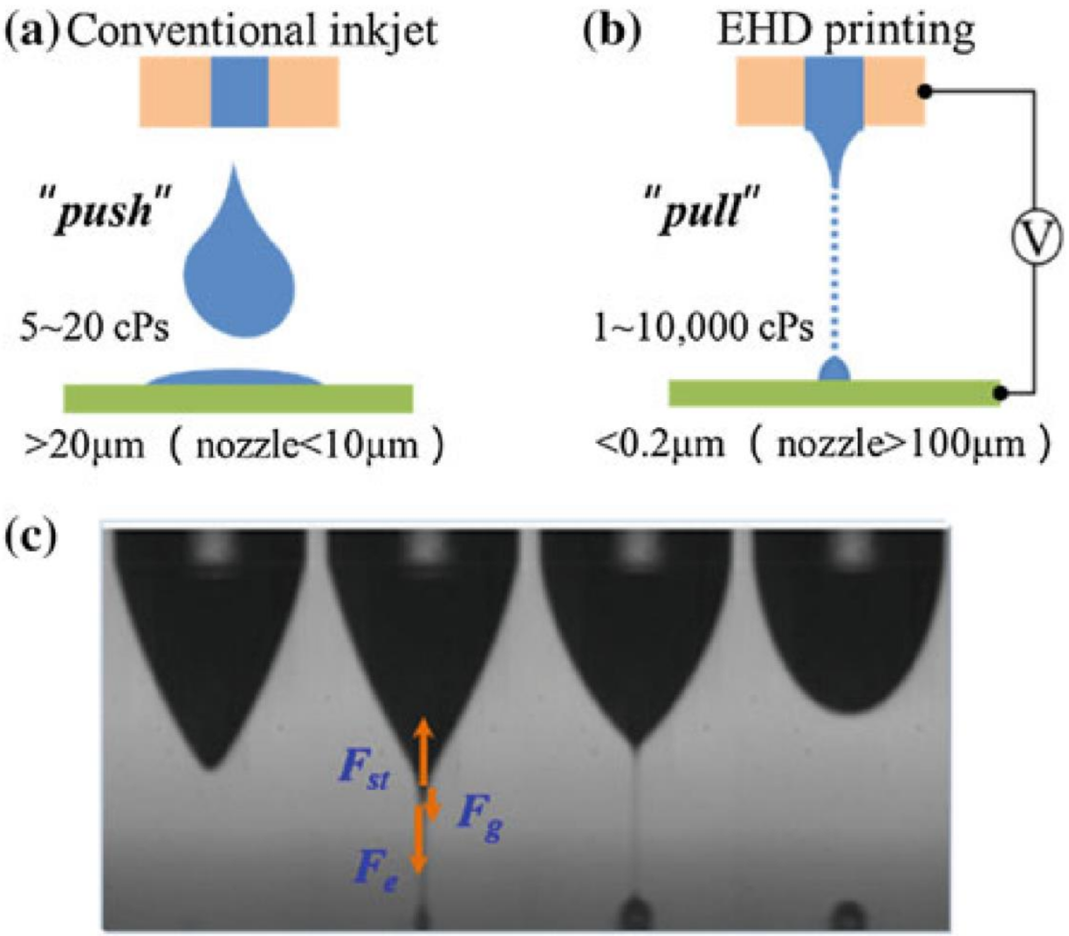


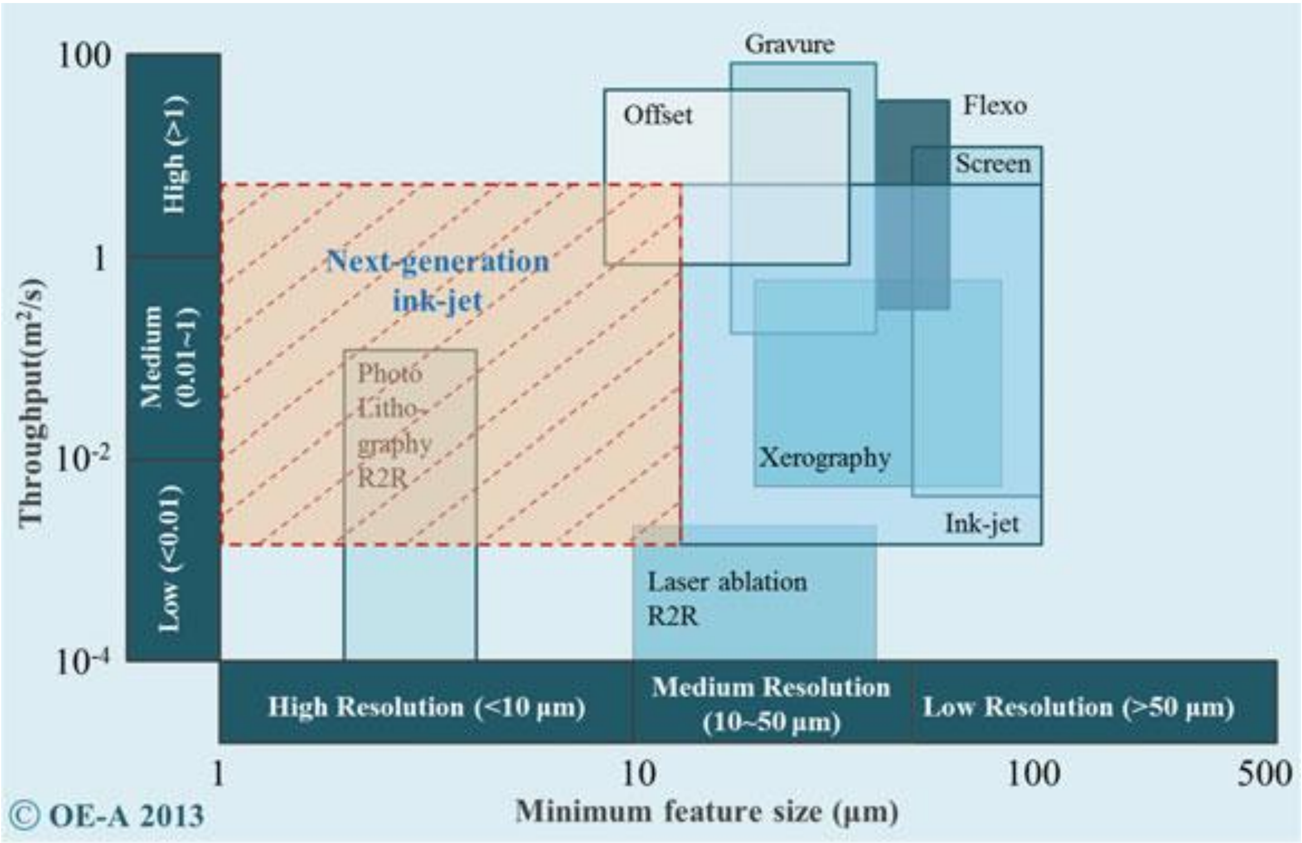
Understanding Rheology
Faith A. Morrison
Oxford University Press (2001)

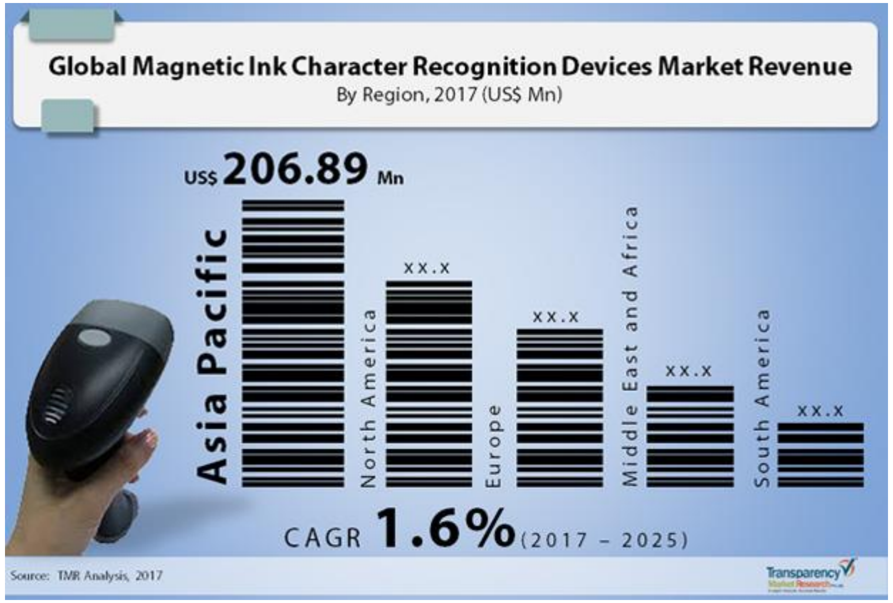
OE-A Roadmap for Organic and Printed Electronics. In: Cantatore E. (eds) Applications of Organic and Printed Electronics. Integrated Circuits and Systems. Springer, Boston, MA. (2013)

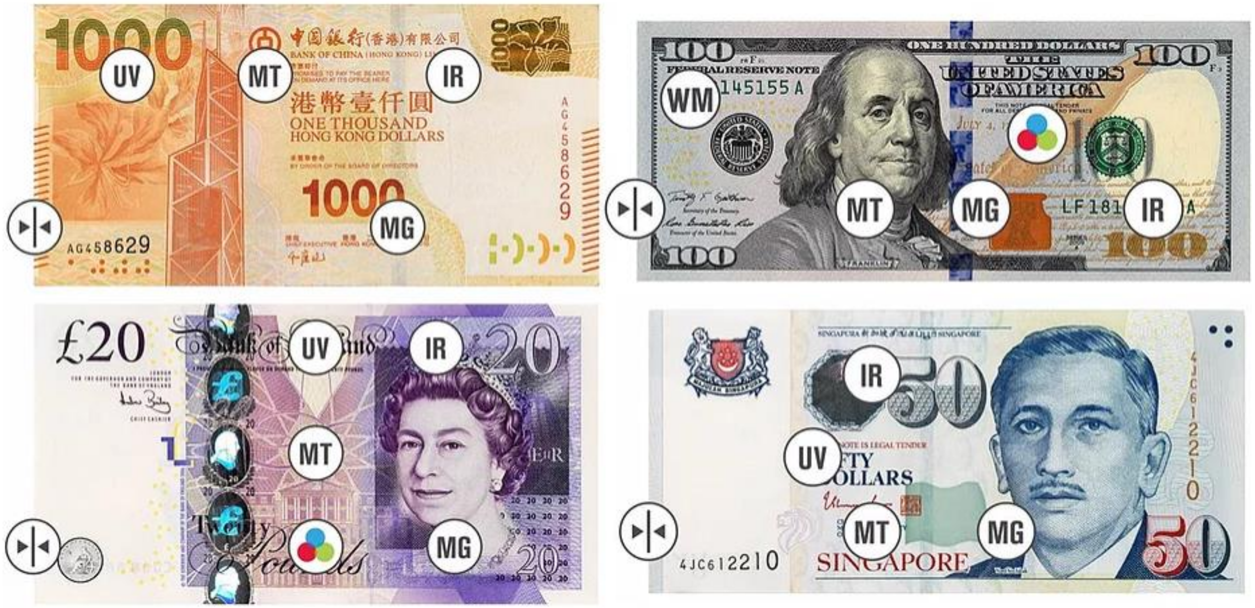
Rheology

Source: Heraeus, manroland, Infineon, Karl Knauer


(a) Conventional inkjet
"push"
5~20 cPs
>20μm (nozzle<10μm)
(b) EHD printing
"pull"
1~10,000 cPs
V
<0.2μm (nozzle>100μm)
(c)
F_st
F_g
F_e


Throughput(m²/s)
100
1
10-2
10-4
High (>1)
Medium (0.01~1)
Low (<0.01)
Gravure
Offset
Flexo
Screen
Next-generation ink-jet
Photo Litho-graphy R2R
Xerography
Ink-jet
Laser ablation R2R
High Resolution (<10 μm)
Medium Resolution (10~50 μm)
Low Resolution (>50 μm)
1
10
100
500
Minimum feature size (μm)
© OE-A 2013


Global Magnetic Ink Character Recognition Devices Market Revenue
By Region, 2017 (US$ Mn)
US$ 206.89 Mn
Asia Pacific
North America
xx.x
Europe
xx.x
Middle East and Africa
xx.x
South America
xx.x
CAGR 1.6% (2017 – 2025)
Source: TMR Analysis, 2017
Transparency Market Research

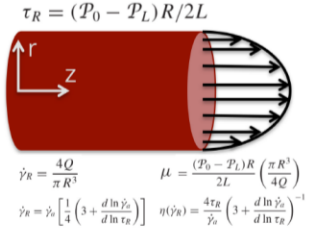

UV
MT
IR
MG
WM

Macro-scale Rheometry

Shear rheometry

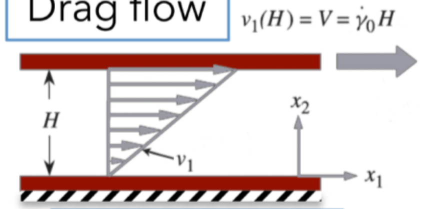
Extensional rheometry

Capillary flow



Capillary rheometers

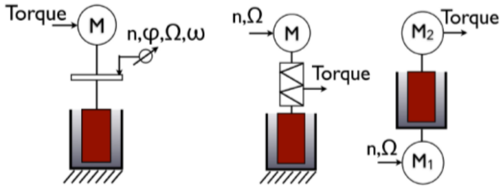
Drag flow



Rotational rheometers

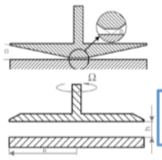
Control Stress

Control Strain



Searle

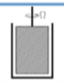
Searle / Couette



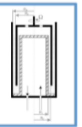
Cone-Plate

Plate-Plate

Concentric cylinders



Double gap concentric cylinders

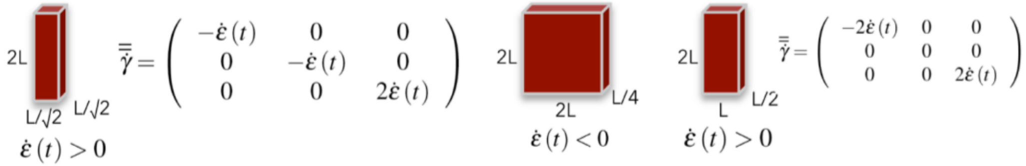


η⇧

Uniaxial extensional flow

Biaxial stretching flow

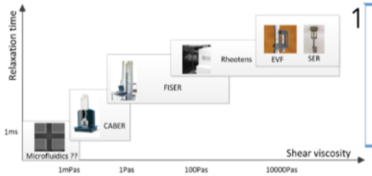
Planar elongational flow



$$\bar{\bar{\dot\gamma}} = \begin{pmatrix} -\dot\varepsilon(t) & 0 & 0 \\ 0 & -\dot\varepsilon(t) & 0 \\ 0 & 0 & 2\dot\varepsilon(t) \end{pmatrix}$$

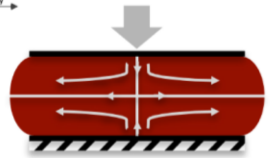
$\dot\varepsilon(t) > 0$ (uniaxial); $\dot\varepsilon(t) < 0$ (biaxial); $\dot\varepsilon(t) > 0$ (planar)

$$\bar{\bar{\dot\gamma}} = \begin{pmatrix} -2\dot\varepsilon(t) & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 2\dot\varepsilon(t) \end{pmatrix}$$

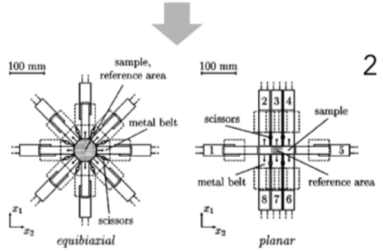


1

Squeeze flow in rotational rheometers



Meissner's rheometers can provide biaxial and planar flows for polymer melts



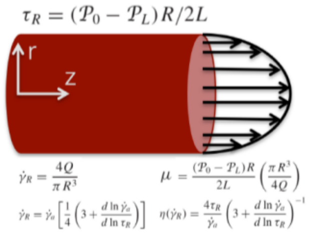
2

F.J. Galindo-Rosales. "Complex fluids and Rheometry in microfluidics". Chapter 1 in Complex fluid-flows in microfluidics, Springer International Publishing (2018).

Macro-scale Rheometry

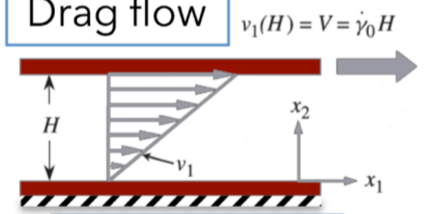
Shear rheometry

Capillary flow



Capillary rheometers

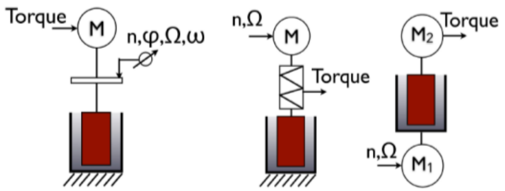
Drag flow



Rotational rheometers

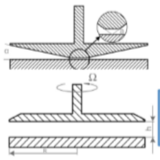
Control Stress

Control Strain



Searle

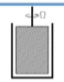
Searle / Couette



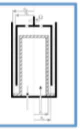
Cone-Plate

Plate-Plate

Concentric cylinders



Double gap concentric cylinders



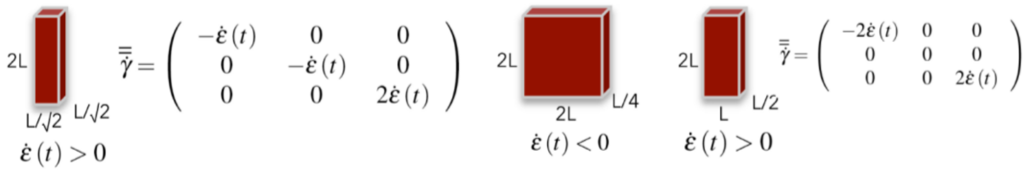
η⇧

Extensional rheometry

Uniaxial extensional flow

Biaxial stretching flow

Planar elongational flow

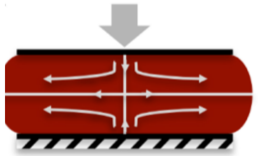


$$\bar{\bar{\dot{\gamma}}} = \begin{pmatrix} -\dot{\varepsilon}(t) & 0 & 0 \\ 0 & -\dot{\varepsilon}(t) & 0 \\ 0 & 0 & 2\dot{\varepsilon}(t) \end{pmatrix}$$

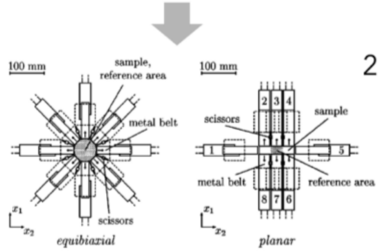
$$\bar{\bar{\dot{\gamma}}} = \begin{pmatrix} -2\dot{\varepsilon}(t) & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 2\dot{\varepsilon}(t) \end{pmatrix}$$

CaBER-1
Thermo Scientific

Squeeze flow in rotational rheometers

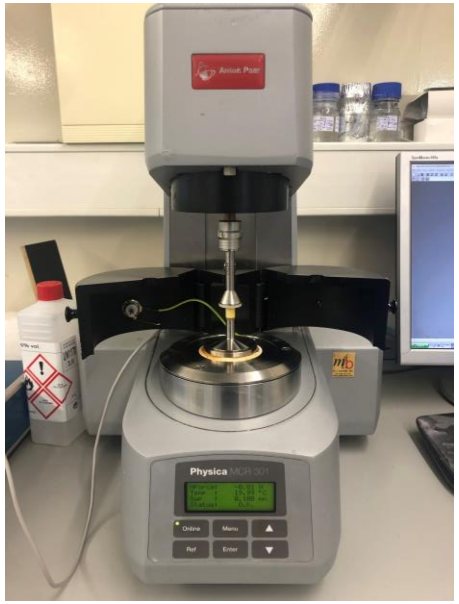


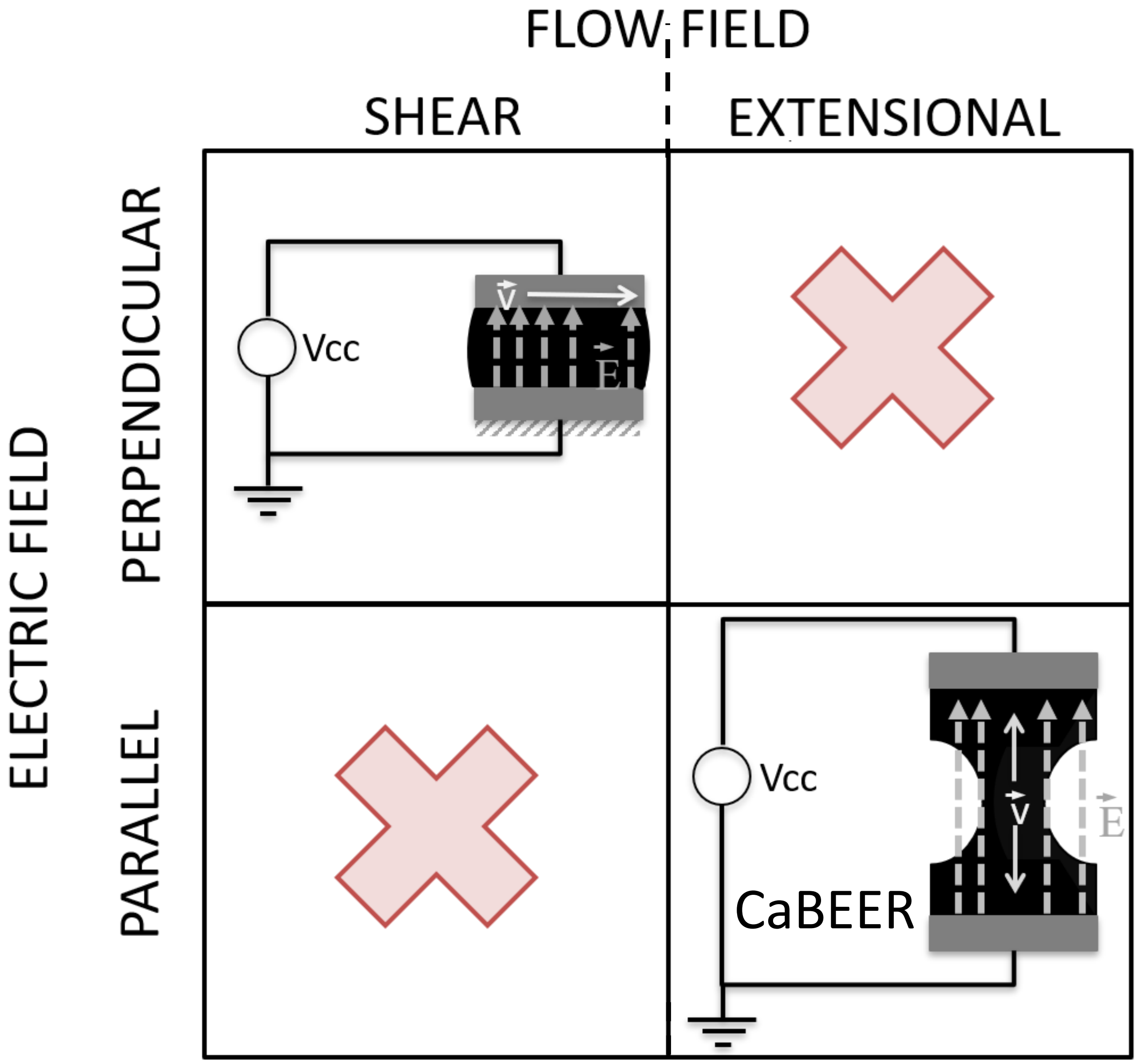
Meissner's rheometers can provide biaxial and planar flows for polymer melts

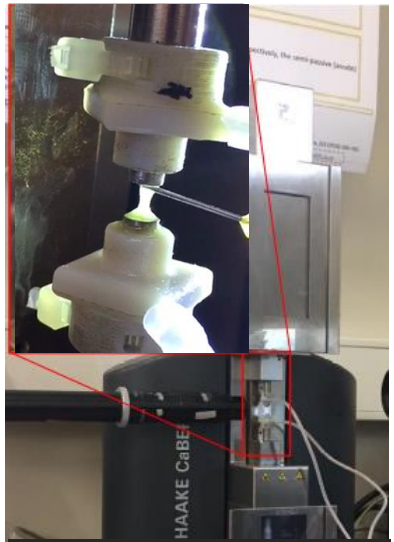


F.J. Galindo-Rosales. "Complex fluids and Rheometry in microfluidics". Chapter 1 in Complex fluid-flows in microfluidics, Springer International Publishing (2018).

CaBEER experiments



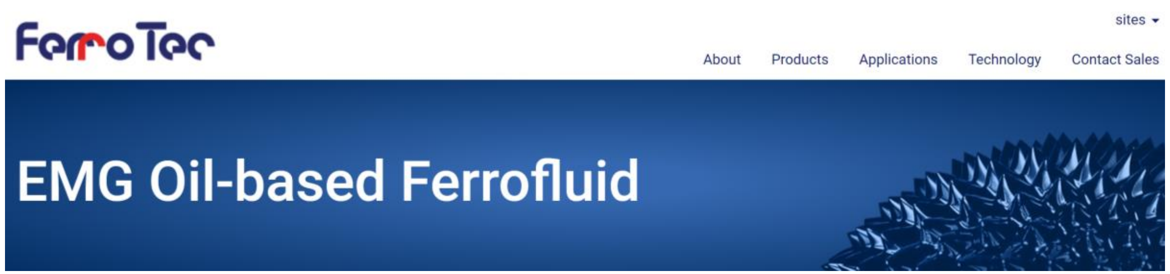


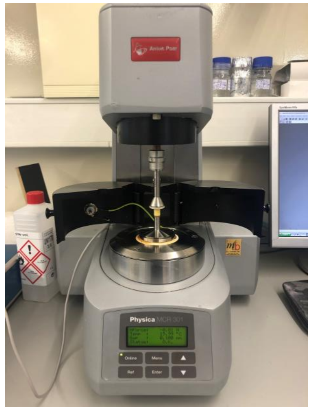


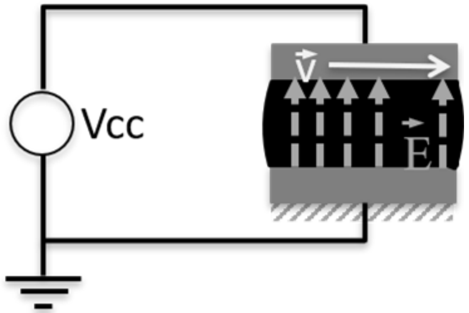
(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)
(19) World Intellectual Property Organization
International Bureau
(43) International Publication Date
15 October 2020 (15.10.2020)
WIPO | PCT
(10) International Publication Number
WO 2020/208550 A1

TRANSPORT PHENOMENA RESEARCH CENTER

COMSOL model for the Capillary Breakup Extensional Electrorheometry (CaBEER) applied to functional inks



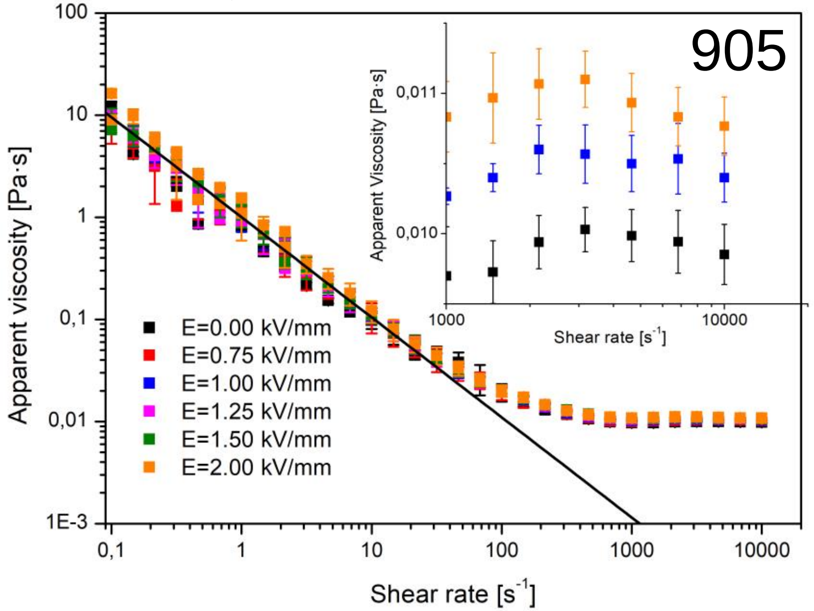


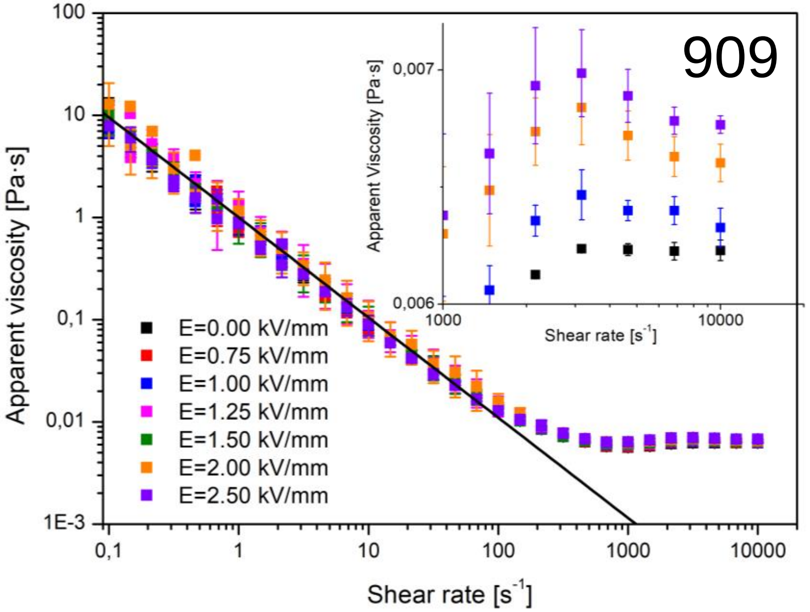


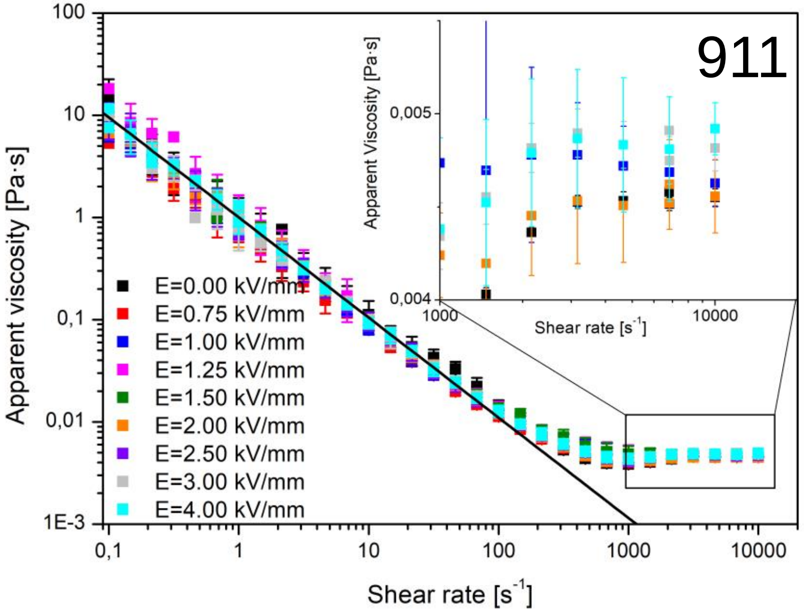
	EMG-905	EMG-909	EMG-911
ρ (kg/m^3) at 25°C	1200	1020	890
η (mPa·s) at 22 °C	9.81 ± 0.07	5.90 ± 0.02	4.04 ± 0.04
σ (mN/m)	22.76	23.66	23.75
a (nm)	~10	~10	~10
Ms (mT)	44	22	11
χ	3.52	1.38	0.50
ϕ (% vol)	7.8	3.9	2

J.H. García-Ortiz and F.J. Galindo-Rosales, JOR (2021) – In preparation
J.H. García-Ortiz and F.J. Galindo-Rosales, IRC (2020)

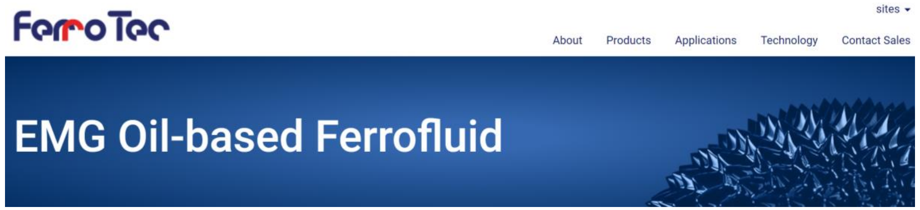
$\varphi(\%vol)$

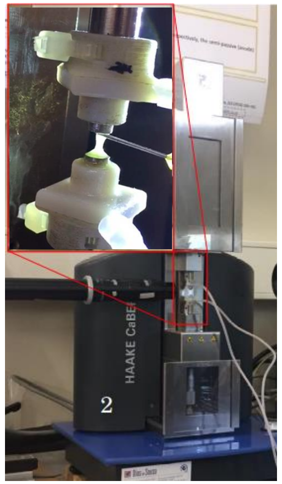


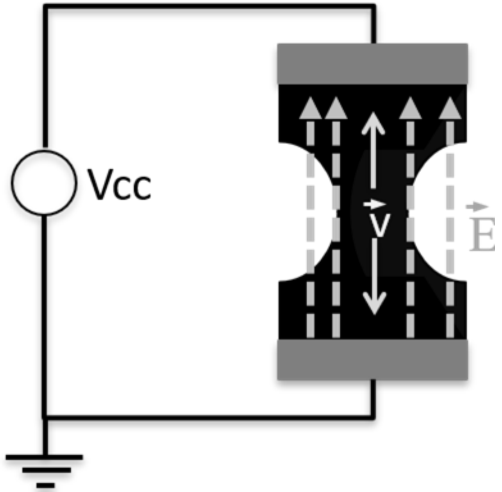




CaBEER experiments



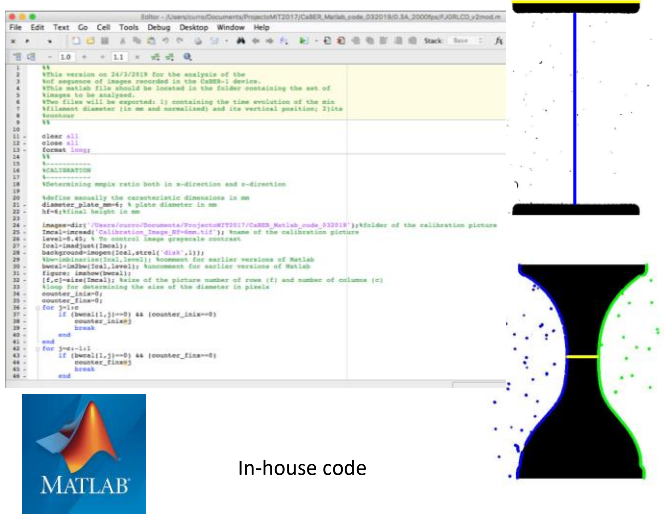




CaBEER

- Slow Retraction Method
- Initial height: 2 mm
- Final height: h_f [mm]
- Plate diameter: 4 mm
- Temperature: 20 ºC

Image post-processing



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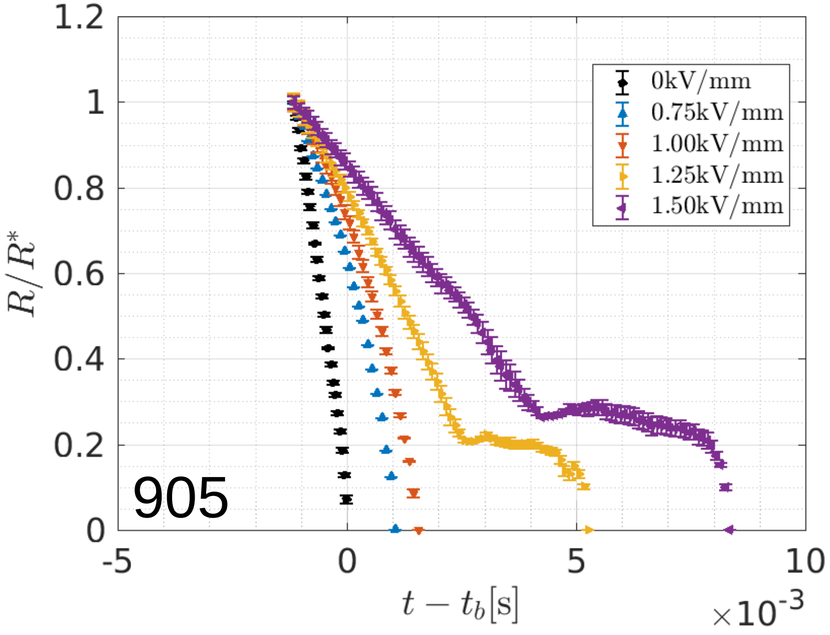
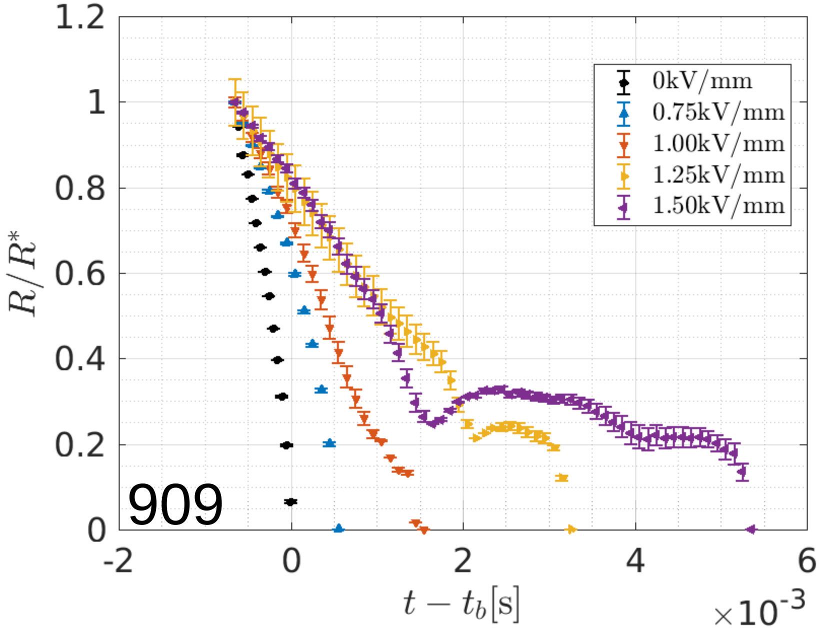
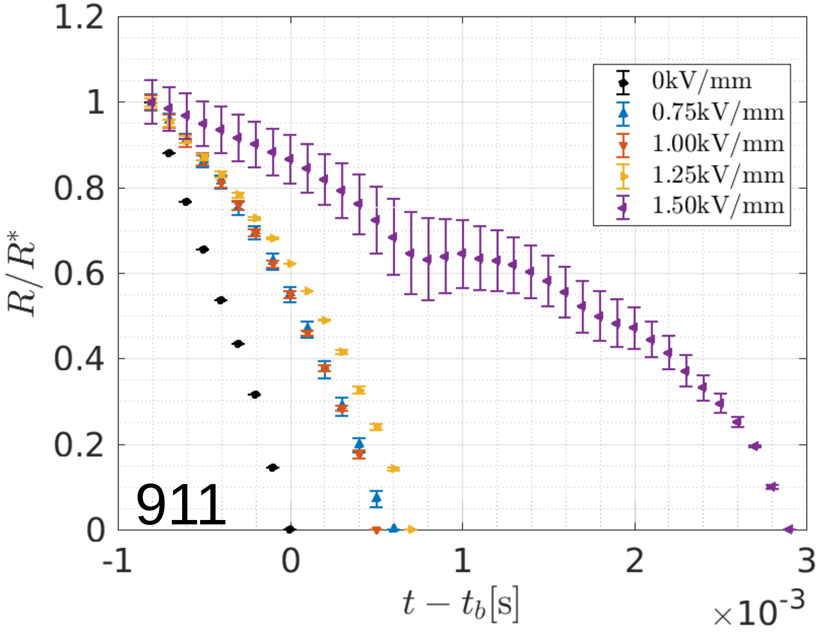
J.H. García-Ortiz and F.J. Galindo-Rosales, IRC (2020)

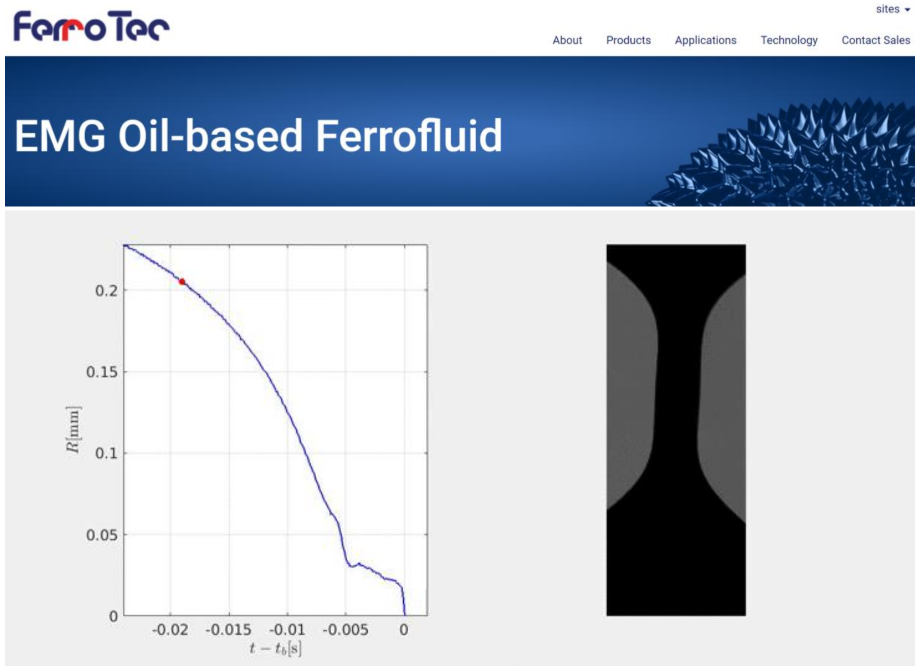
$\varphi(\%vol)$

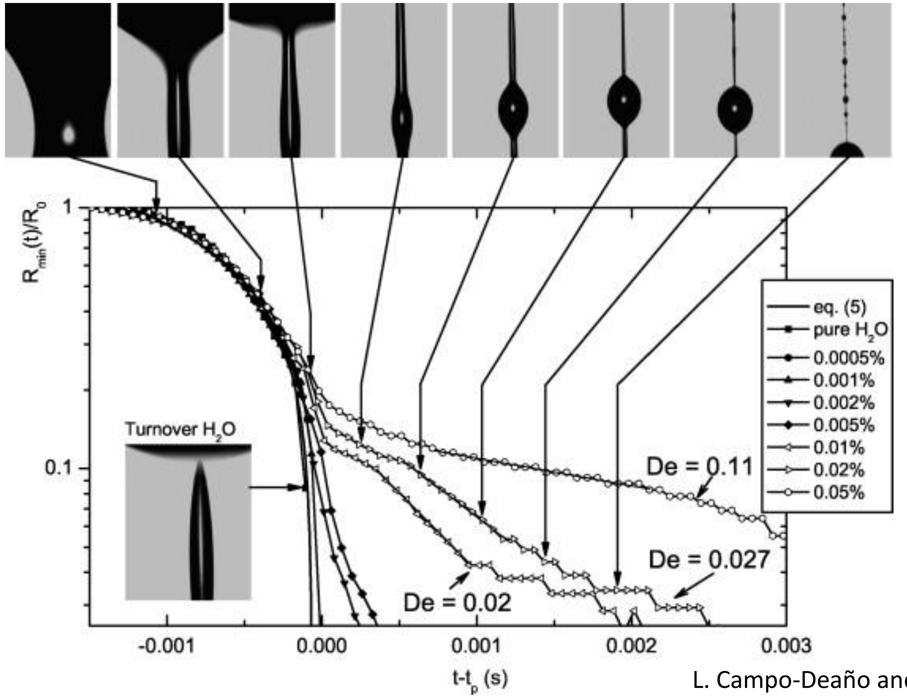






CaBEER experiments





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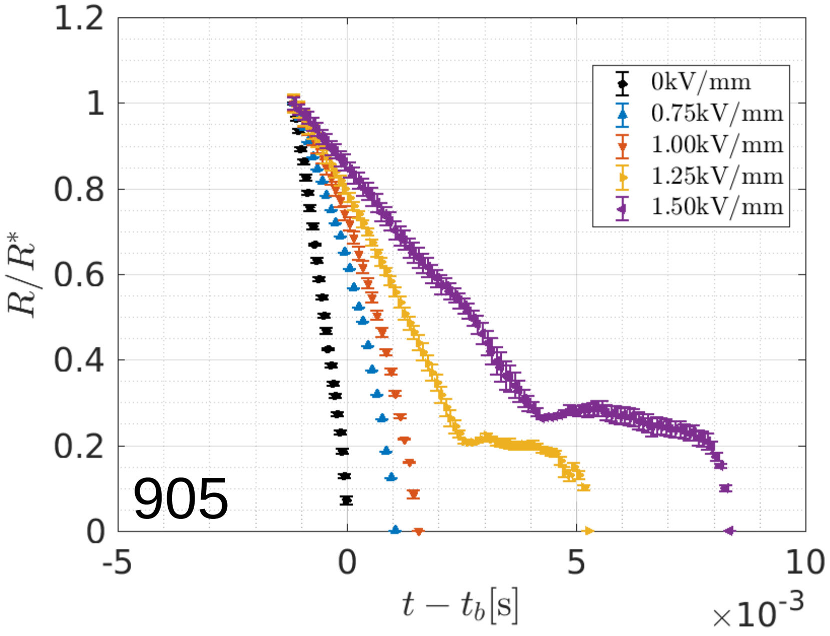
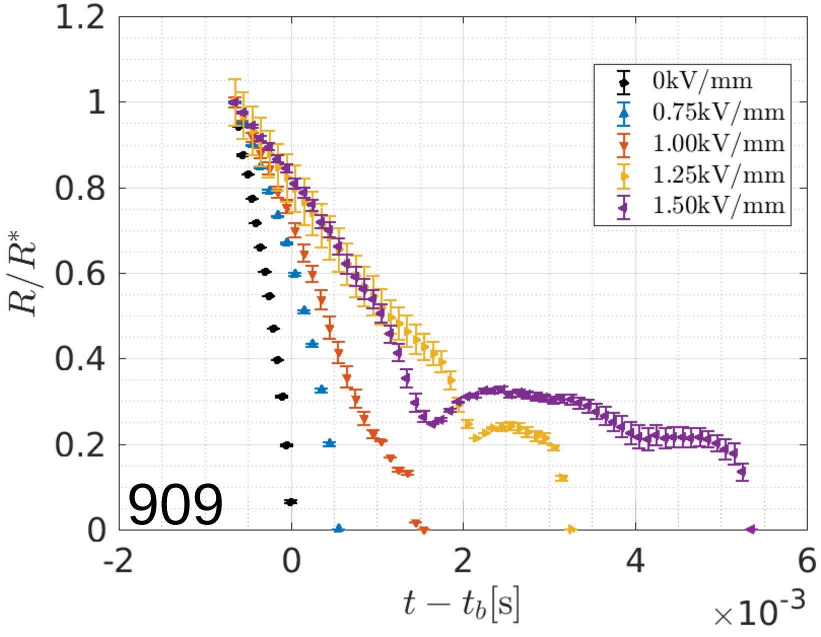
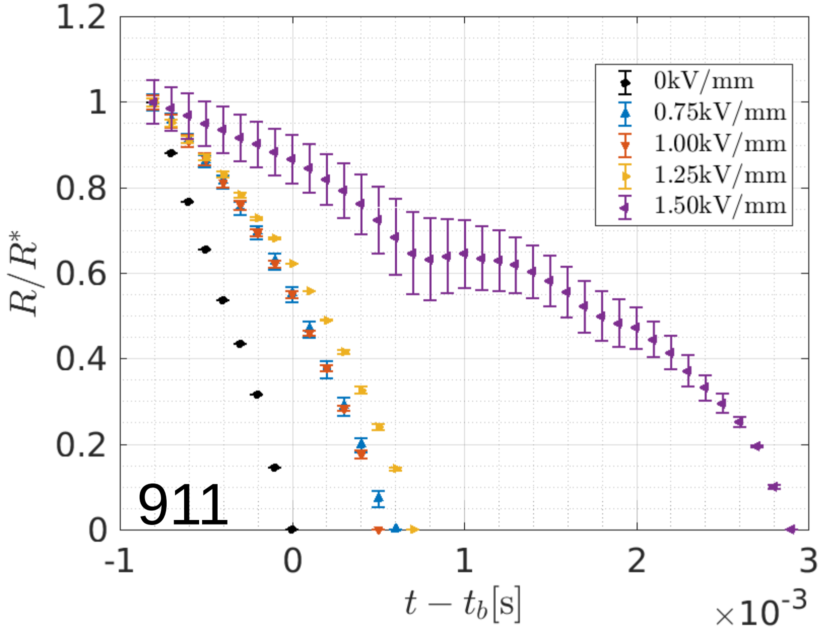
J.H. García-Ortiz and F.J. Galindo-Rosales, IRC (2020)

L. Campo-Deaño and C. Clasen.
JNNFM, 165(23-24):1688–1699, 2010.

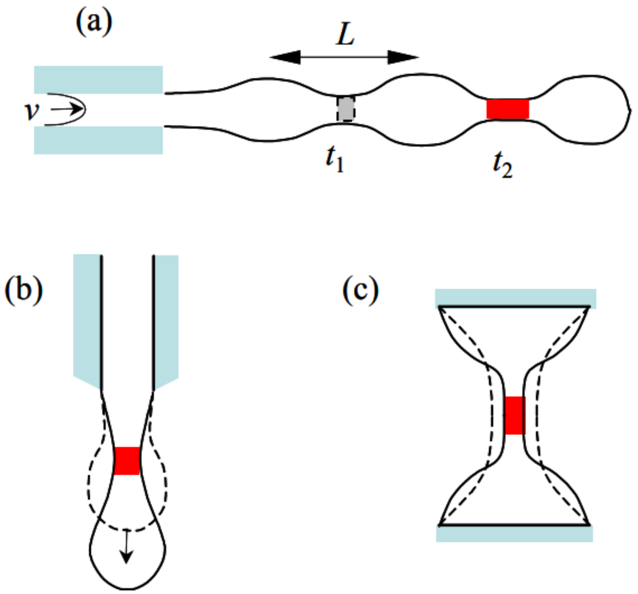
$\varphi(\%vol)$







$$Oh = \frac{\mu}{\sqrt{\rho\sigma R}}$$



Gareth H. Mckinley. Visco-elasto-capillary thinning and break-up of complex fluids. ANNUAL RHEOLOGY REVIEWS, pages 1–49, 2005.

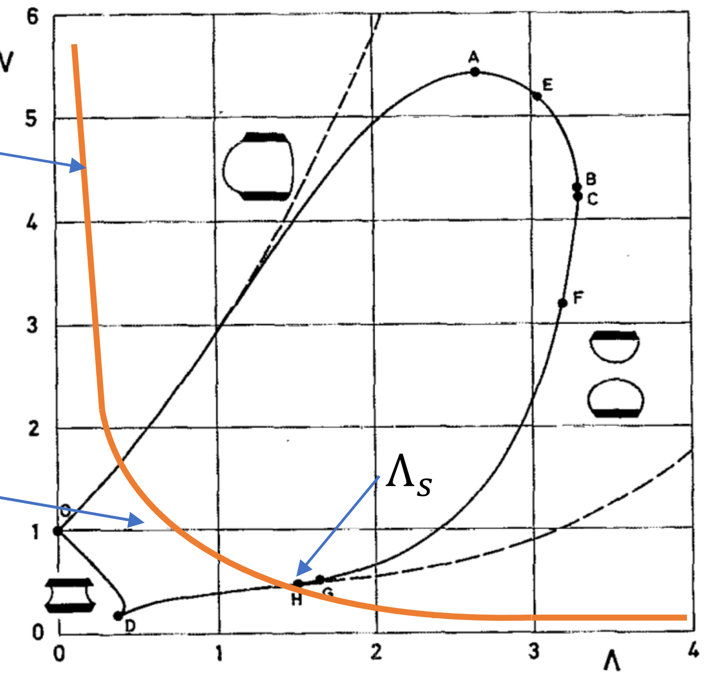
$$\Lambda = \frac{L}{d}$$

$$V = \frac{4V_0}{\pi D_0^{\,3}\Lambda}$$

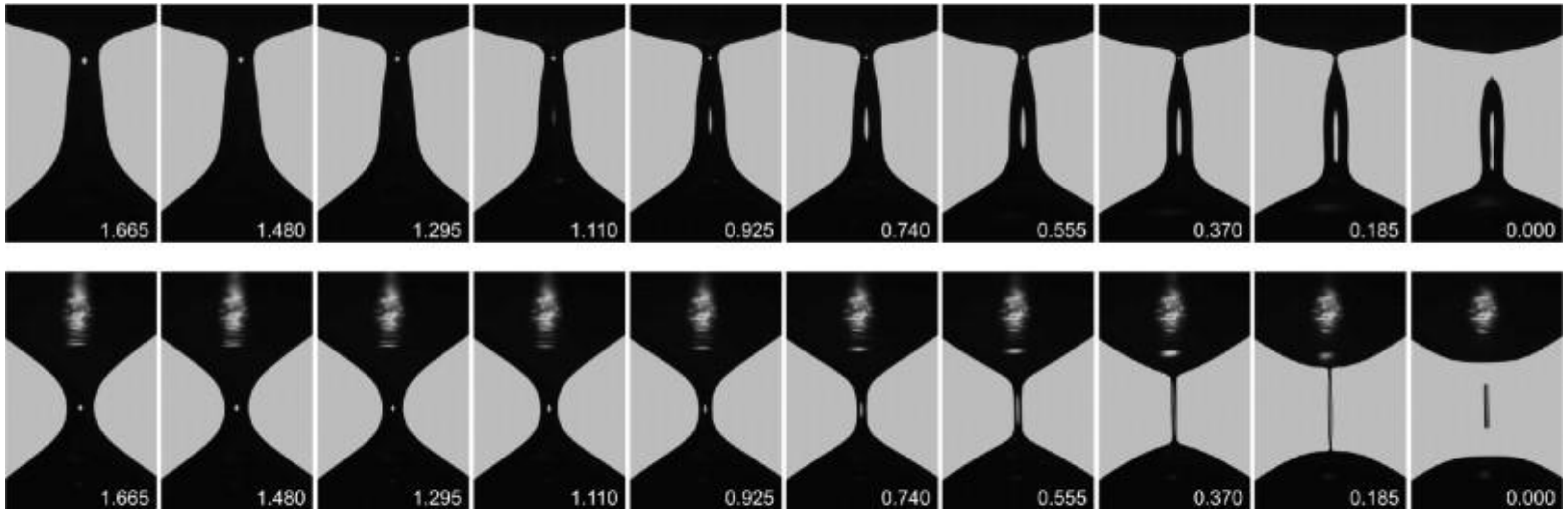
$$Bo = \frac{\rho g R}{2\sigma}$$

Λ_0

Λ_s

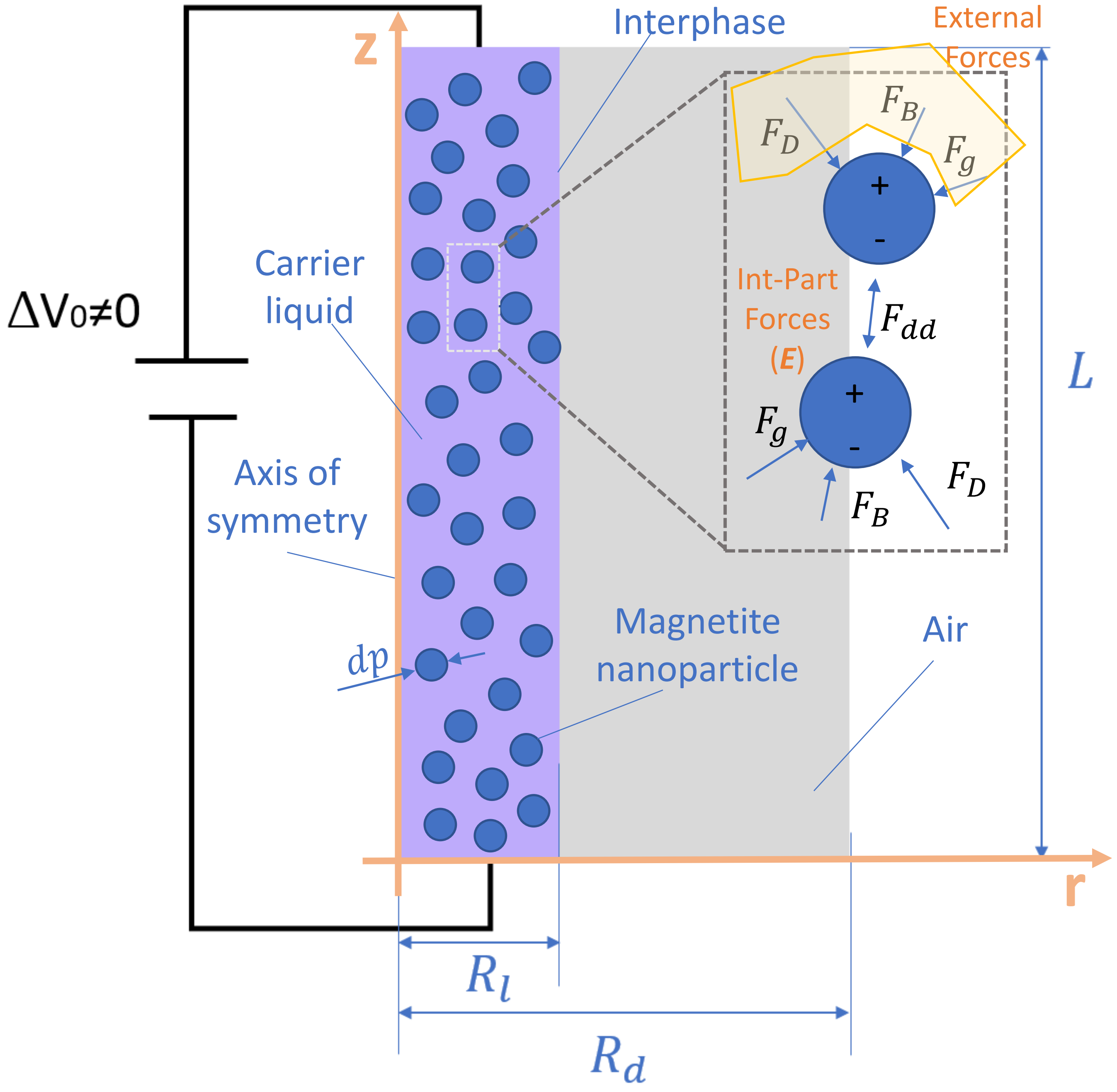


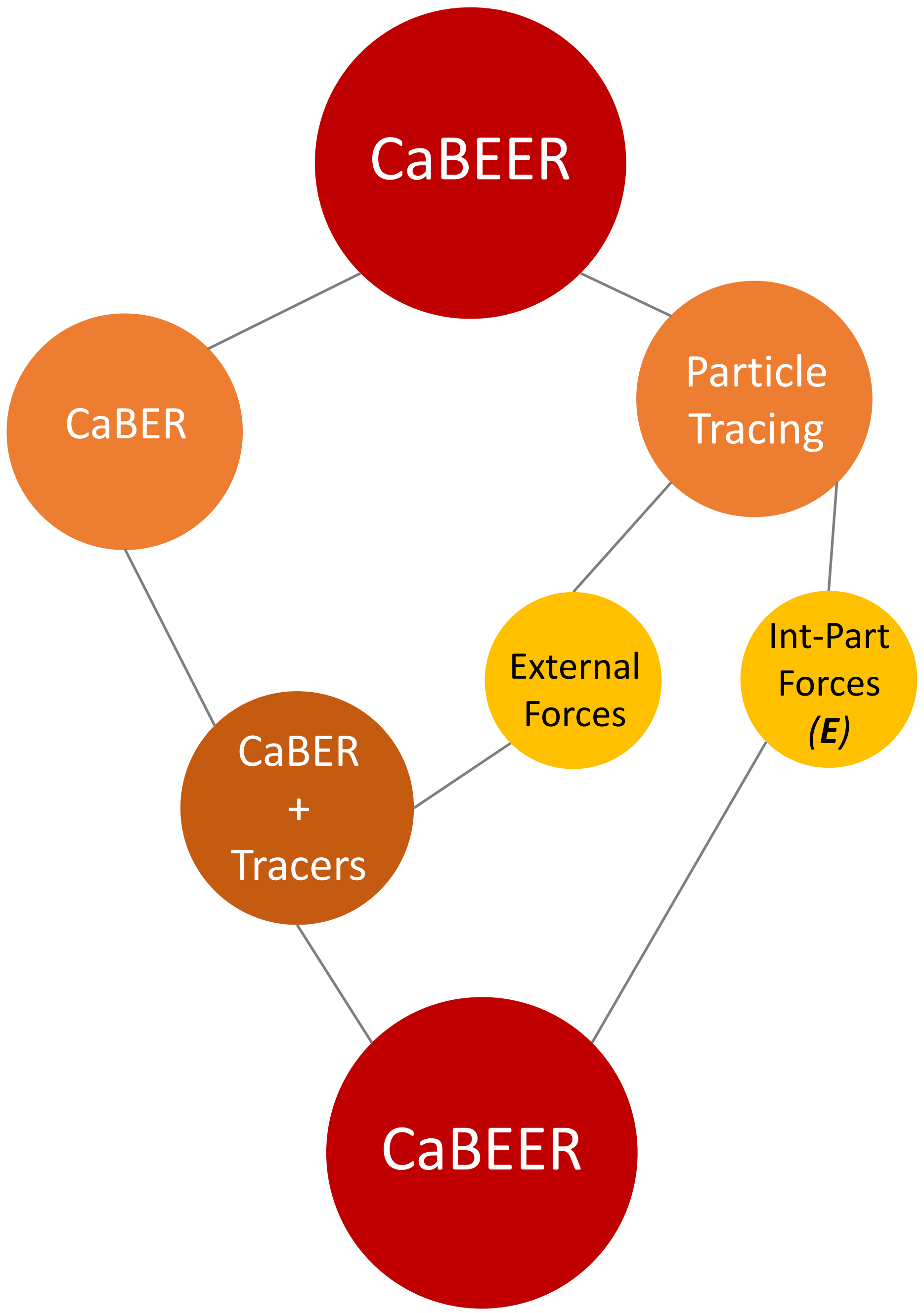
L.A. Slobozhanin and J.M. Perales. Stability of liquid bridges between equal disks in an axial gravity field. PHYSICS OF FLUIDS, A: Fluid Dynamics, 5(6):1305–1314, 1993.



L. Campo-Deaño and C. Clasen.
The slow retraction method (SRM) for the determination of ultra-short relaxation times in capillary breakup extensional rheometry experiments.
JNNFM, 165(23-24):1688–1699, 2010.

Modelling


Interphase
External Forces
F_B
F_D
F_g
Int-Part Forces (*E*)
F_{dd}
L
$\Delta V_0 \neq 0$
Carrier liquid
Axis of symmetry
dp
Magnetite nanoparticle
Air
z
r
R_l
R_d

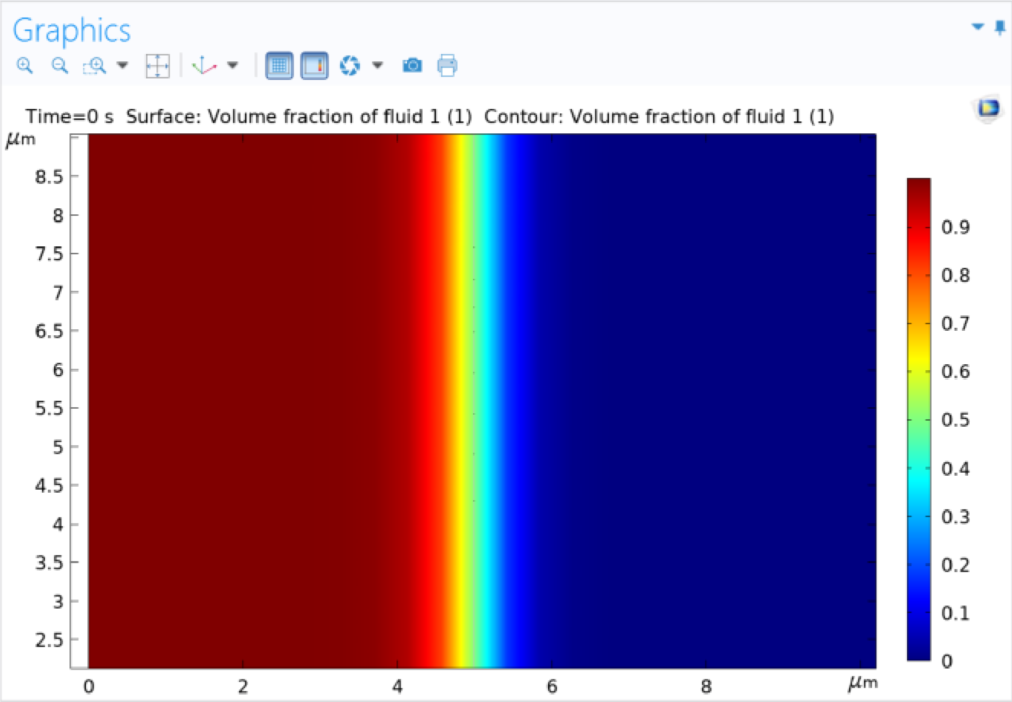

CaBEER
CaBER
Particle Tracing
External Forces
Int-Part Forces (*E*)
CaBER + Tracers
CaBEER

Implementation

Two Phase Flow, phase field

1. Topology changes are expected.

2. Surface tension effects are important.



Laminar flow

$$\nabla \cdot \boldsymbol{v} = 0,$$

$$\rho \frac{\partial v}{\partial t} + \rho (\boldsymbol{v} \cdot \nabla) \boldsymbol{v} = \nabla \cdot \left[-p\boldsymbol{I} + \mu \left(\nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^T \right) + \right] + \boldsymbol{F_{st}} + \rho \boldsymbol{g}$$

Phase field method

$$\frac{\partial \Phi}{\partial t} + \boldsymbol{v} \cdot \nabla \Phi = \nabla \cdot \frac{\gamma \lambda}{\epsilon^2} \nabla \Psi,$$

$$\Psi = -\nabla \cdot \epsilon^2 \nabla \Phi + (\Phi^2 - 1)\Phi + \left(\frac{\epsilon^2}{\lambda} \right) \frac{\partial f_{ext}}{\partial \Phi}$$

$$\sigma = \frac{2\sqrt{2}}{3} \frac{\lambda}{\epsilon}$$

$$\gamma = \chi \epsilon^2$$

$$G = \lambda \left(-\nabla^2 \Phi + \frac{\Phi(\Phi^2 - 1)}{\epsilon^2} \right) + \frac{\partial f}{\partial \Phi}$$

$$V_f = min(max([1 + \Phi)/2], 0), 1)$$

$$\boldsymbol{F_{st}} = \left(G - \frac{\partial f}{\partial \Phi} \right) \nabla \Phi$$

$$\rho = \rho_l + (\rho_l - \rho_g) V_f$$

$$\mu = \mu_l + (\mu_l - \mu_g) V_f$$

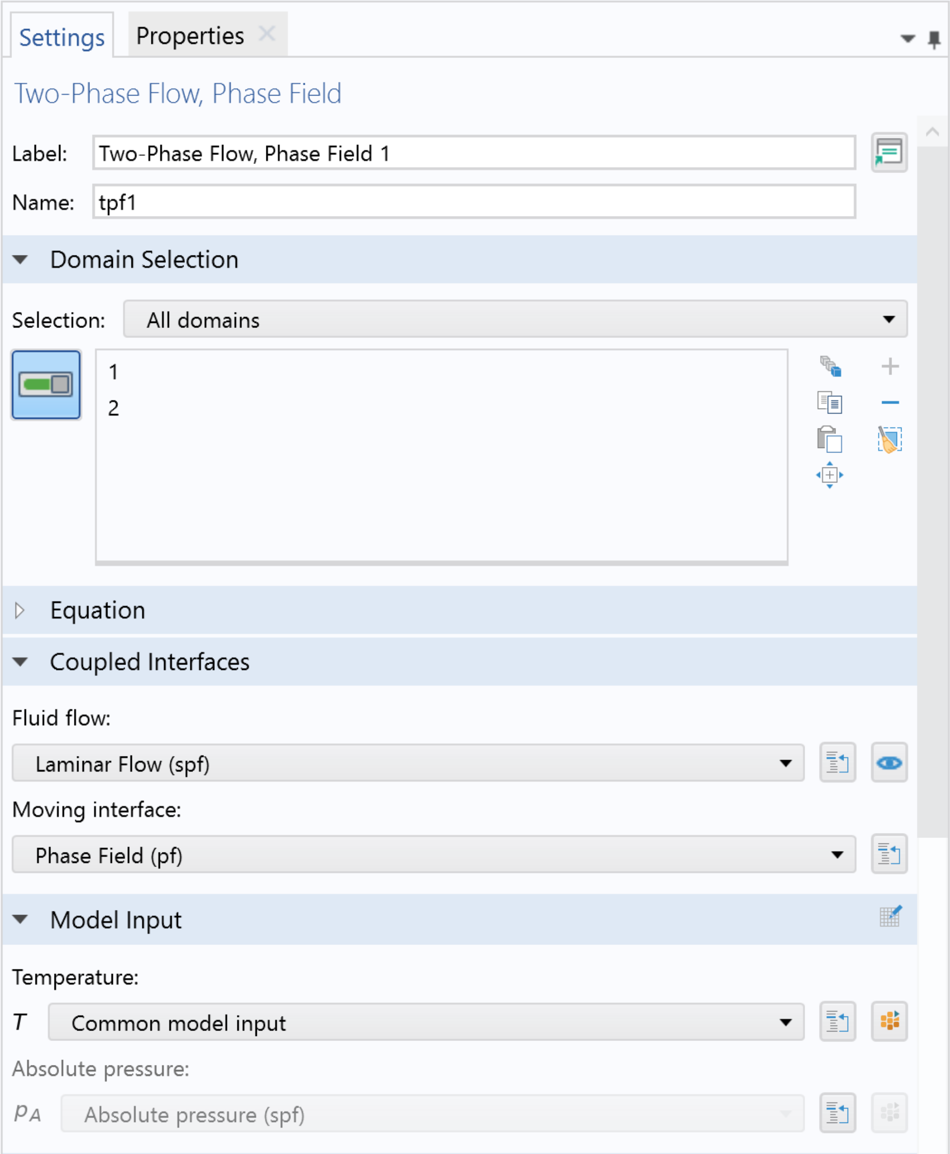
$$\epsilon = \epsilon_l + (\epsilon_l - \epsilon_g) V_f$$

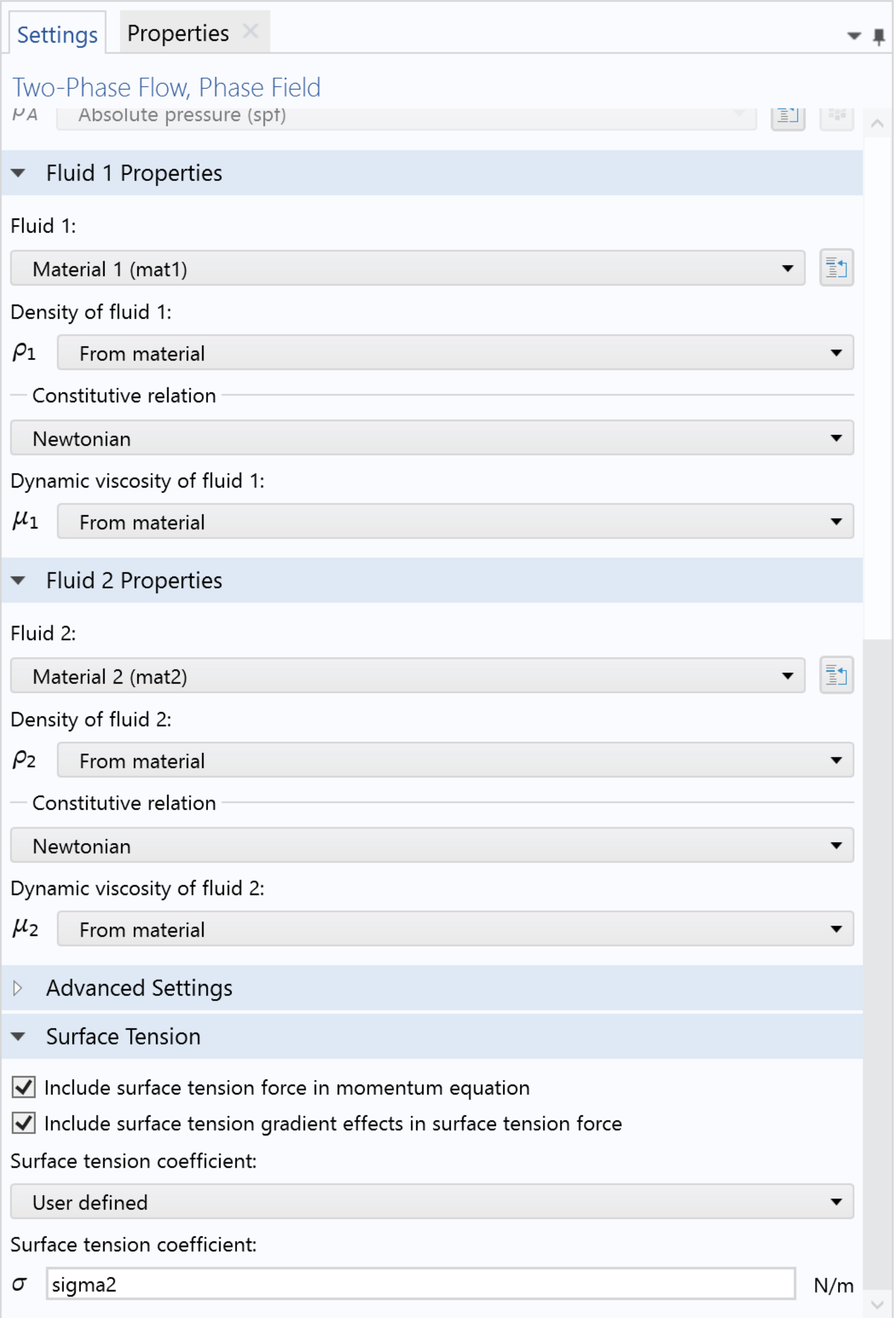
$$\kappa = 2(1 + \Phi)(1 - \Phi) \frac{G}{\sigma}$$

$$G = \lambda \left(-\nabla^2 \Phi + \frac{\Phi(\Phi^2 - 1)}{\epsilon^2} \right) + \frac{\partial f}{\partial \Phi}$$

Two Phase Flow, phase field

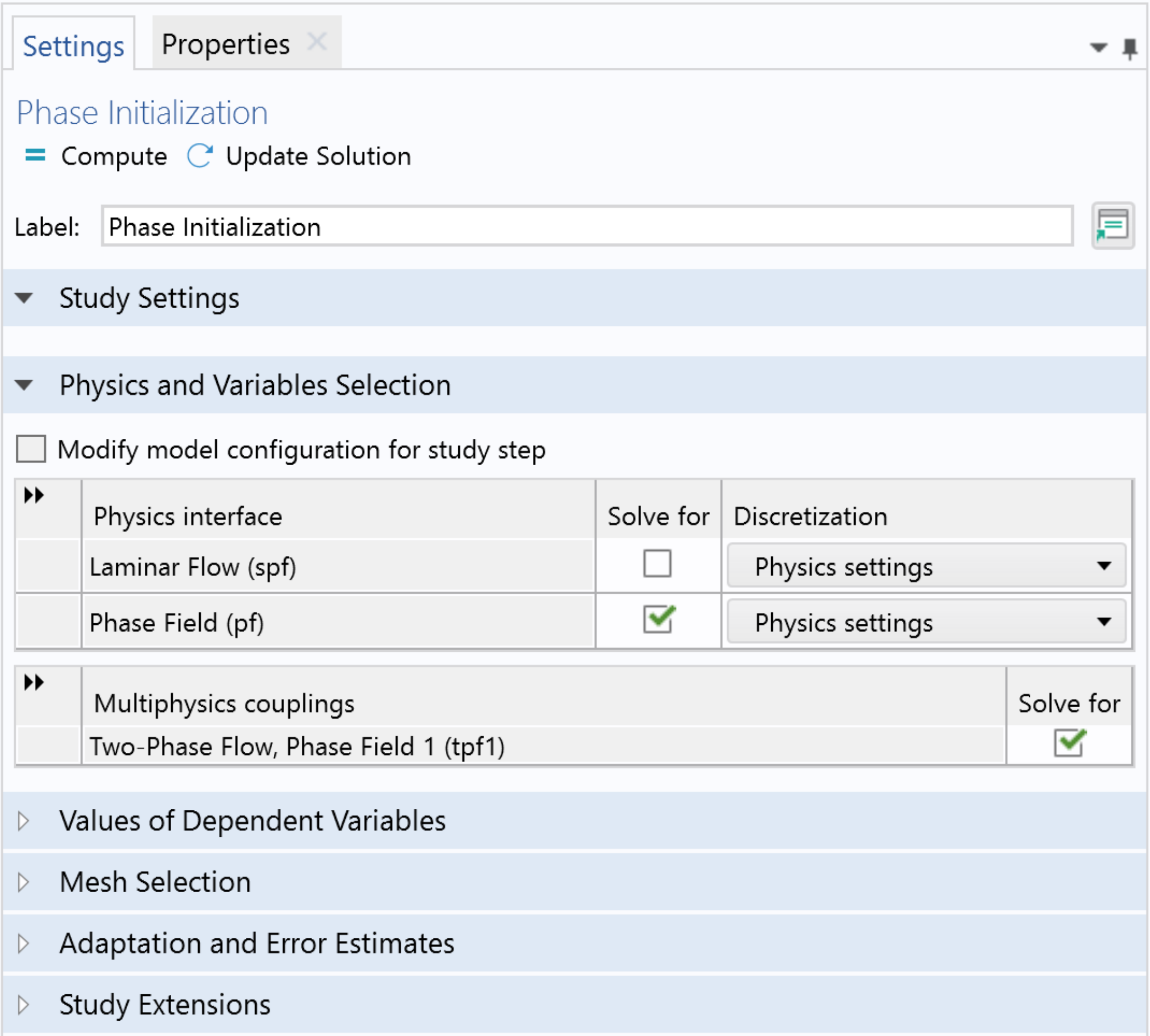
Implementation

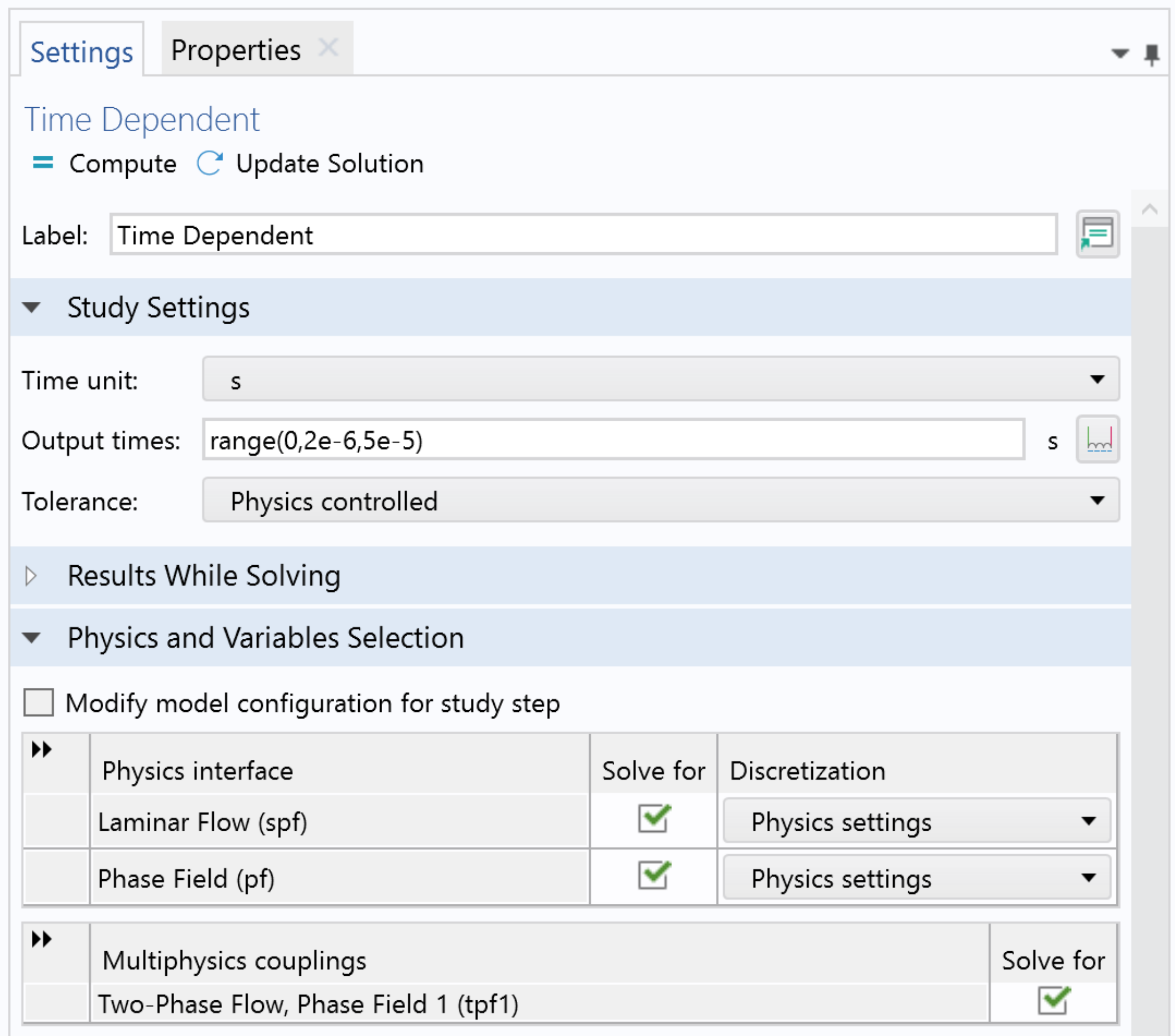




Two Phase Flow, phase field

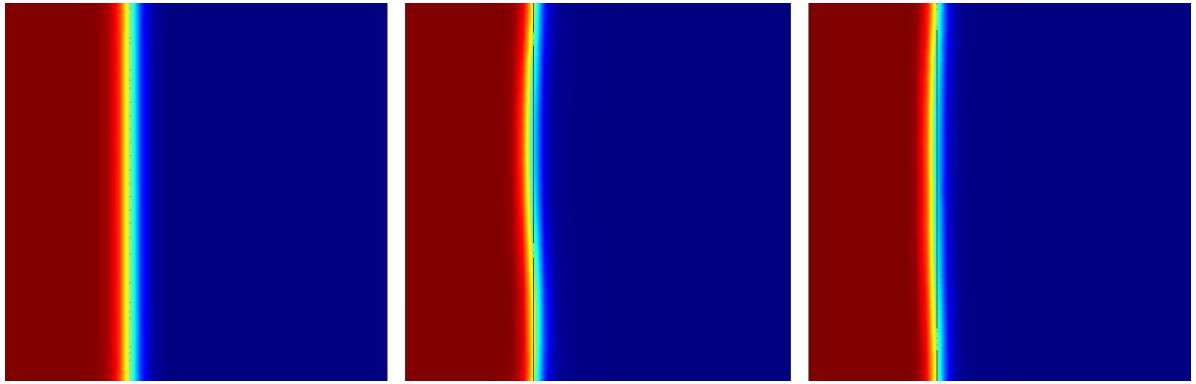
Implementation





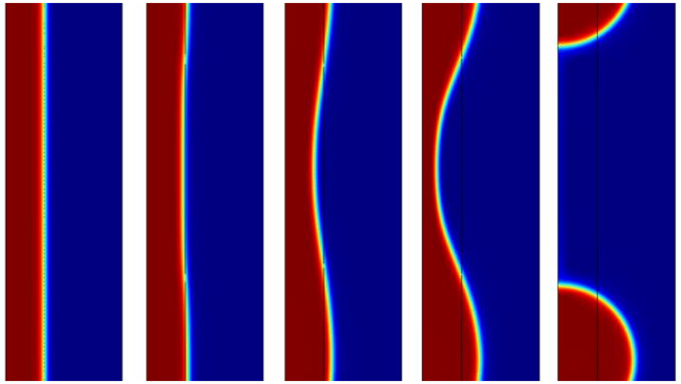
Results: CaBEERTwoPhaseFlow.mph

Two Phase Flow, phase field



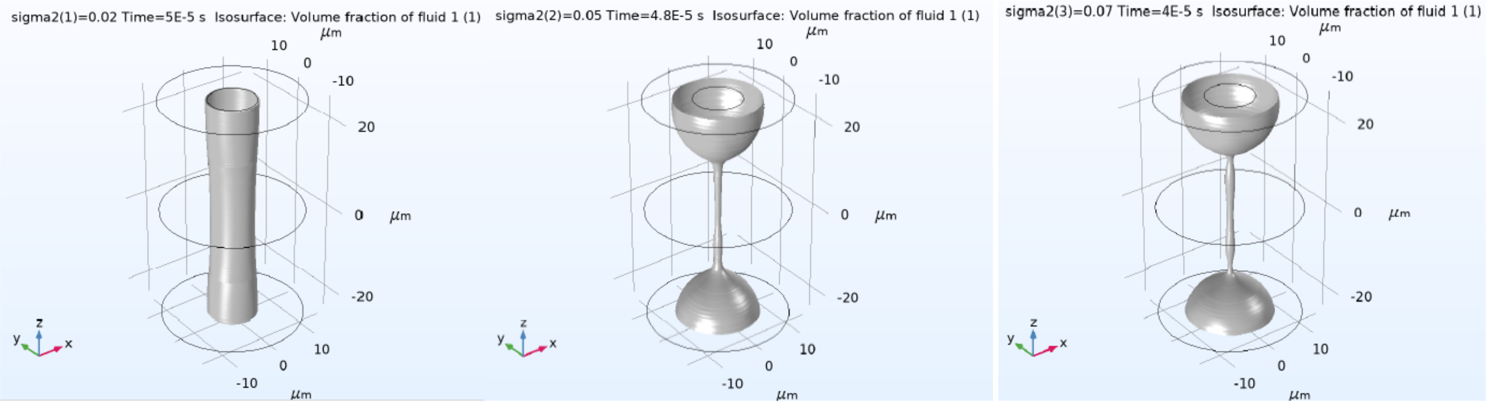
$1\ ms$

$\Lambda_1 = 1.5$



$0.14\ ms$

$\Lambda_2 = 5$



(a) $\sigma = 0.02$ (b) $\sigma = 0.05$ (c) $\sigma = 0.07$

Particle Tracing for Fluid Flow

External forces

Brownian force (F_B)

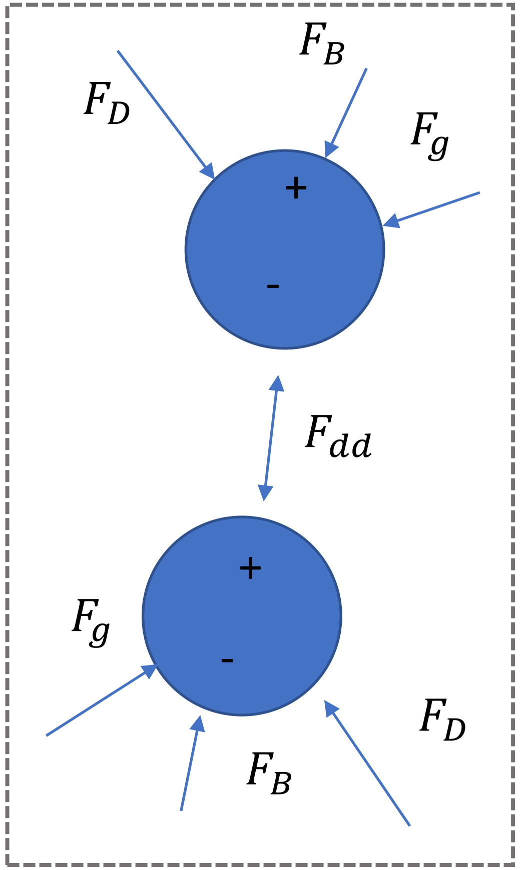
$$F_B = \zeta \sqrt{\frac{6\pi k_B \mu T d_p}{\Delta t}}$$

Drag force (F_D)

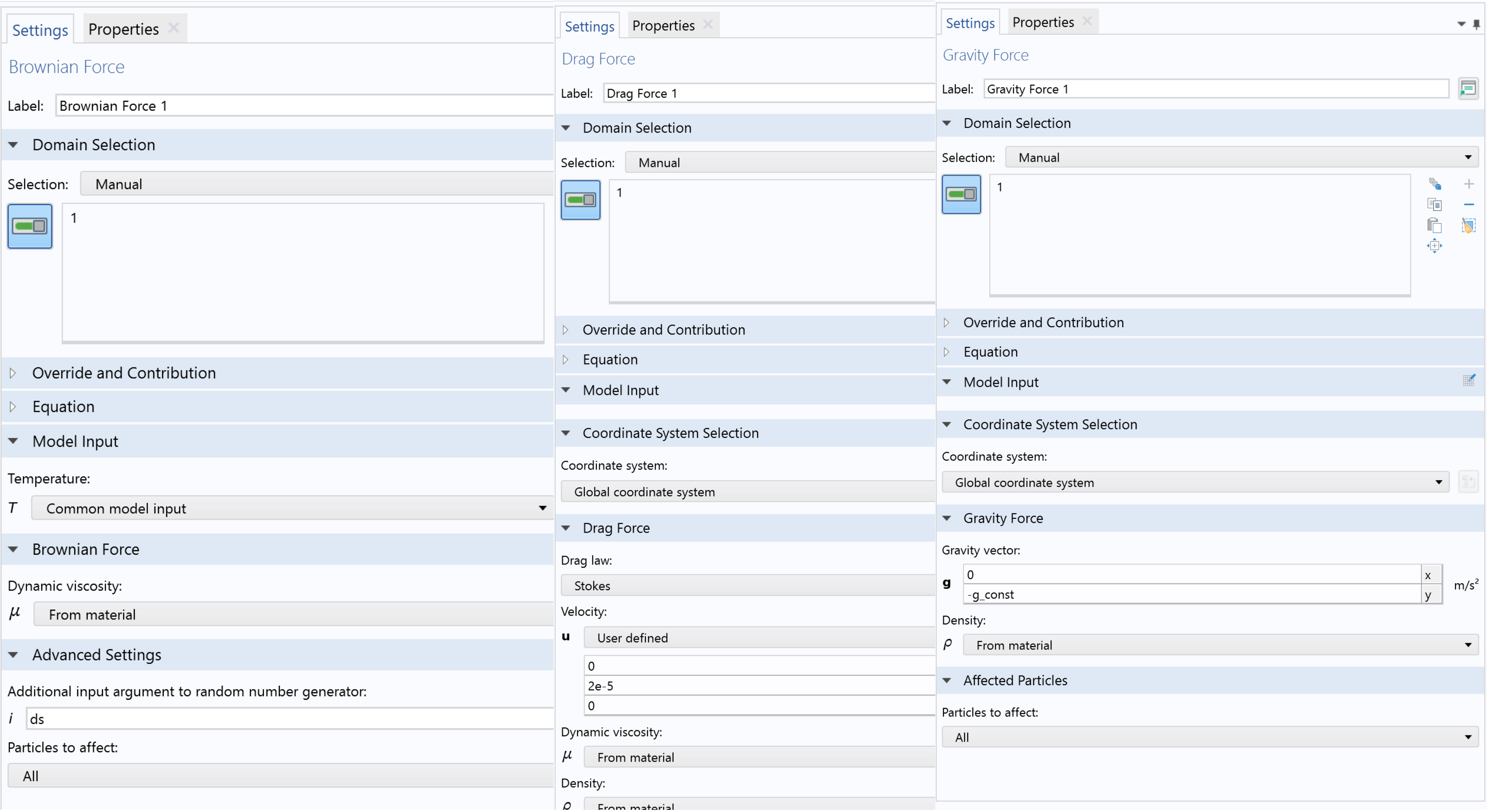
$$F_D = 3\pi\mu d_p (u - v)$$

Gravitational force (F_g)

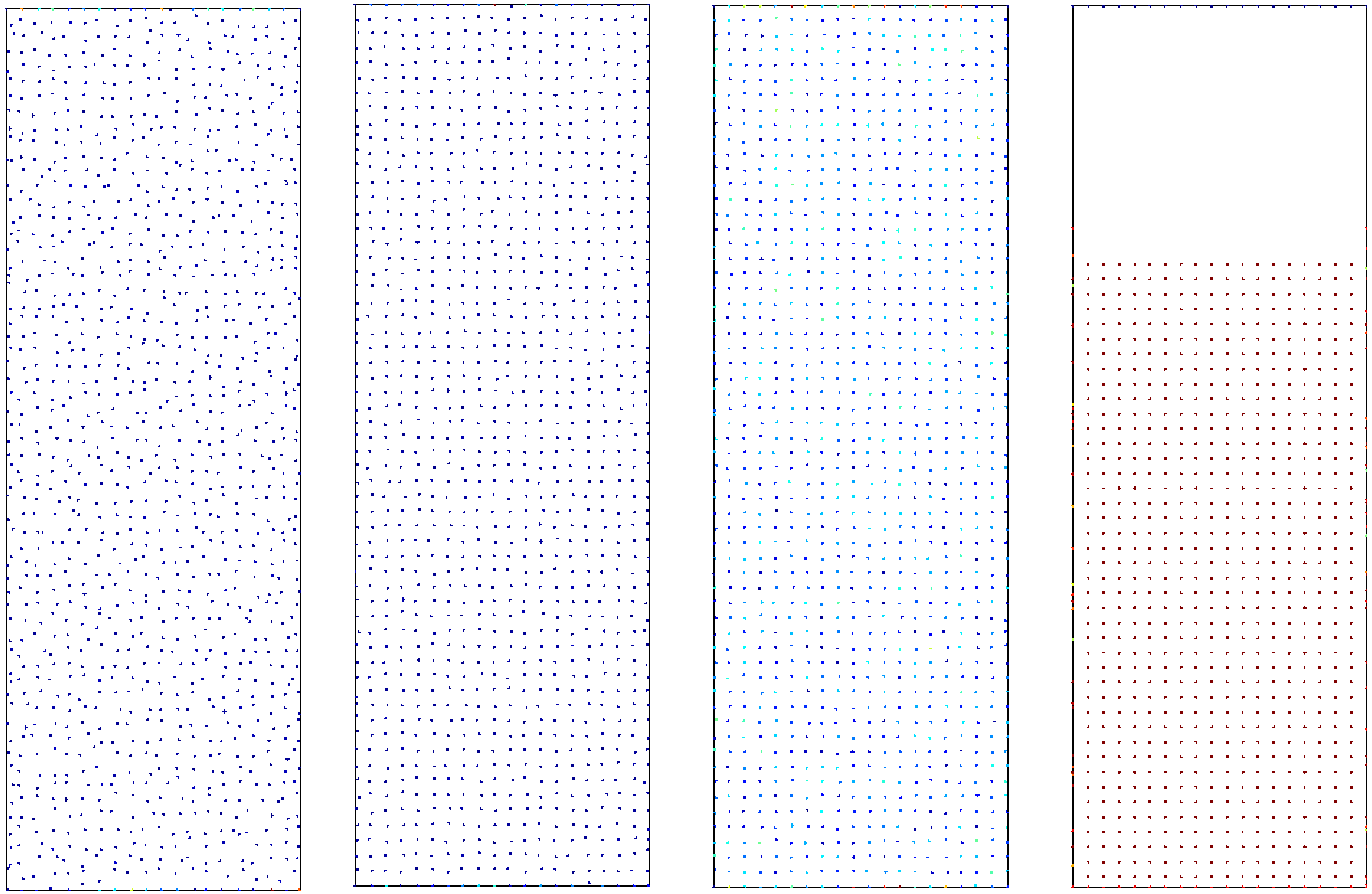
$$F_g = \frac{(\rho_p - \rho_l)\pi d_p^3}{6} g$$



Particle Tracing for Fluid Flow – External forces



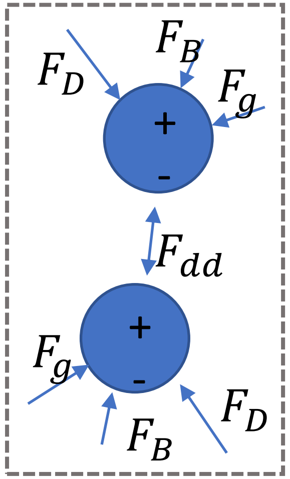
Particle Tracing for Fluid Flow – External forces



$$r_p = \{100\ nm, 500\ nm, 1\ \mu m, 500\ \mu m\}$$

Particle Tracing for Fluid Flow

Inter-particle force



Inter-particle force ($\boldsymbol{F}_{dd}$)

$$\boldsymbol{F}_{dd} = \frac{15\left(\boldsymbol{p}_1 \cdot \boldsymbol{r}\right)\left(\boldsymbol{p}_2 \cdot \boldsymbol{r}\right)}{4\pi\epsilon_0 r^7}\boldsymbol{r} - \frac{3\left[\boldsymbol{p}_1\left(\boldsymbol{p}_2 \cdot \boldsymbol{r}\right) + \boldsymbol{p}_2\left(\boldsymbol{p}_1 \cdot \boldsymbol{r}\right) + \boldsymbol{r}\left(\boldsymbol{p}_1 \cdot \boldsymbol{p}_2\right)\right]}{4\pi\epsilon_0 r^5}$$

Electrostatic

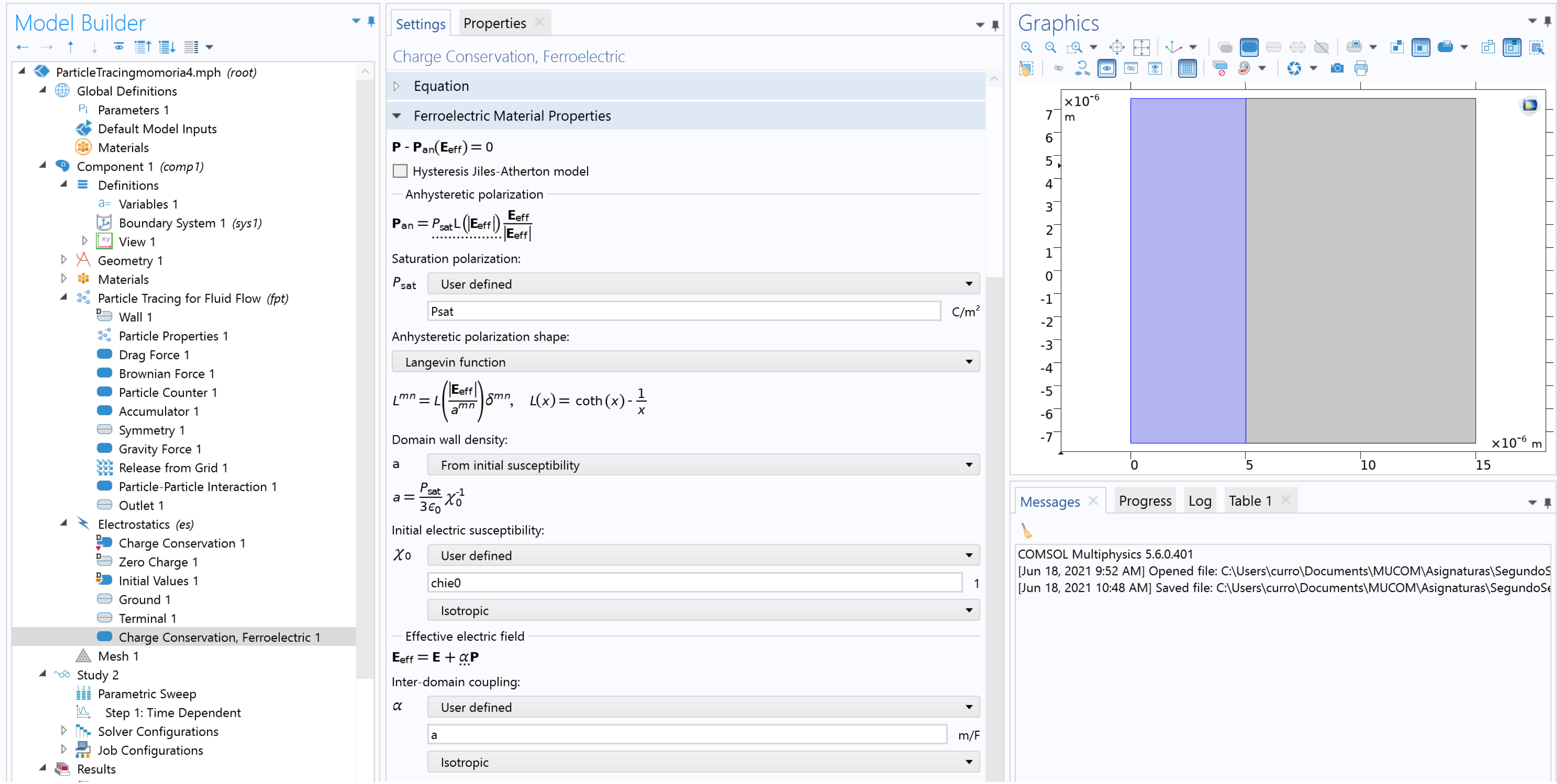
$$-\nabla \cdot \left(\epsilon_0 \nabla V - \boldsymbol{P}\right) = \rho_c$$

$$\boldsymbol{P} = P_S L\left(|\boldsymbol{E}_{eff}|\right)\frac{\boldsymbol{E}_{eff}}{|\boldsymbol{E}_{eff}|}$$

$$\boldsymbol{E}_{eff} = \boldsymbol{E} + \alpha \boldsymbol{P}$$

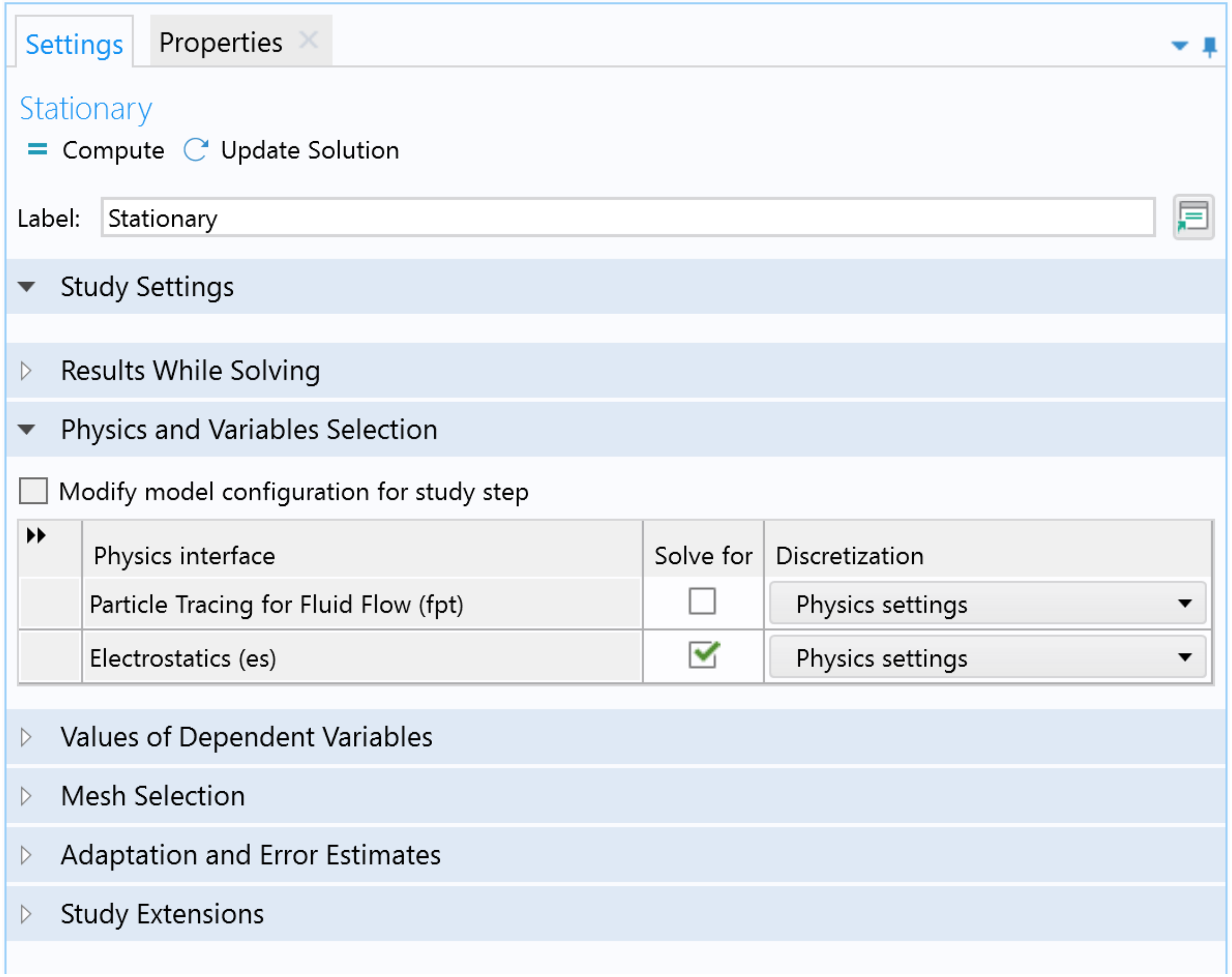
$$L = coth\left(\frac{3\chi_0|\boldsymbol{E}_{eff}|}{P_s}\right) - \frac{P_s}{3\chi_0|\boldsymbol{E}_{eff}|}$$

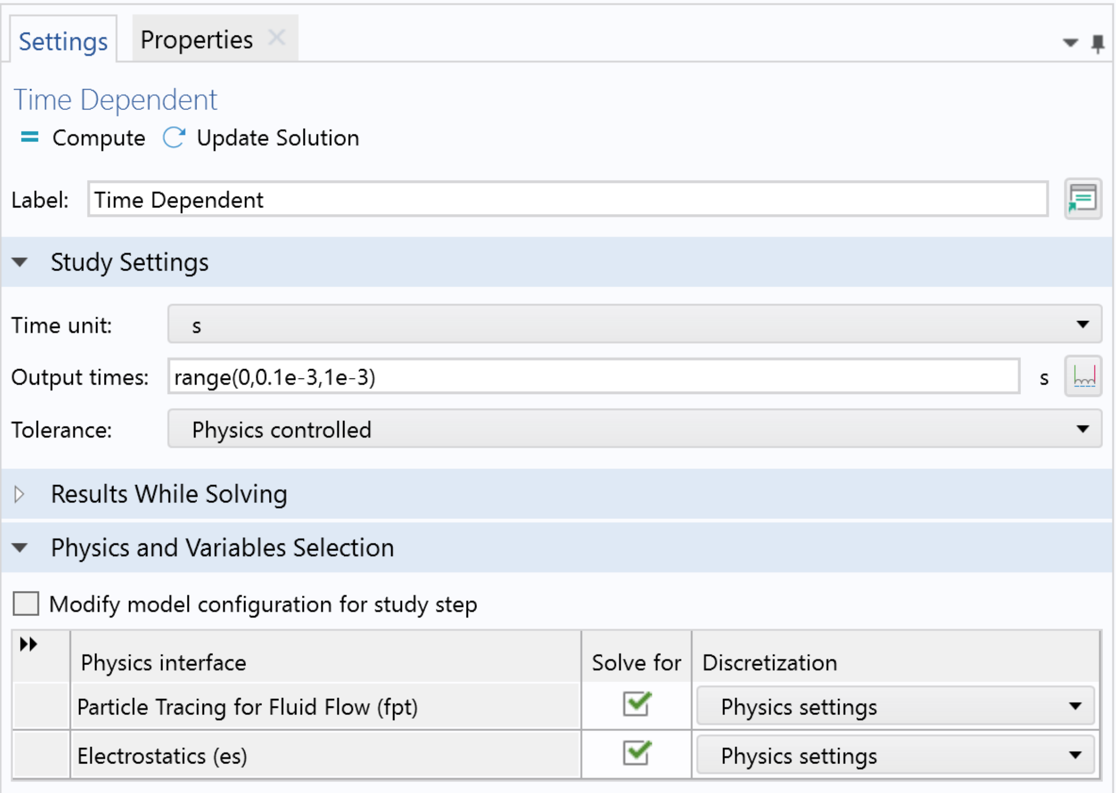
Particle Tracing for Fluid Flow – Interparticle force



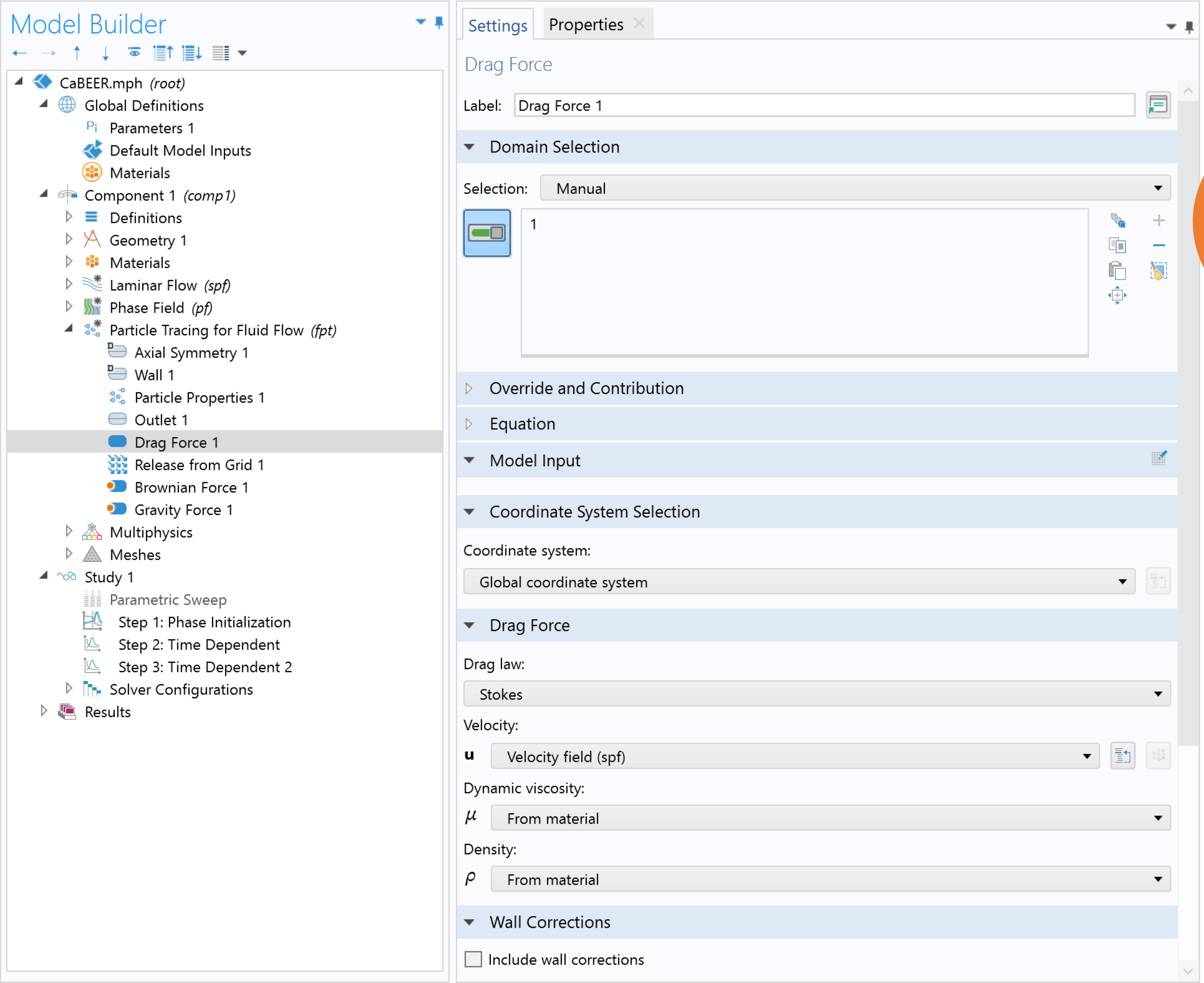
Implementation

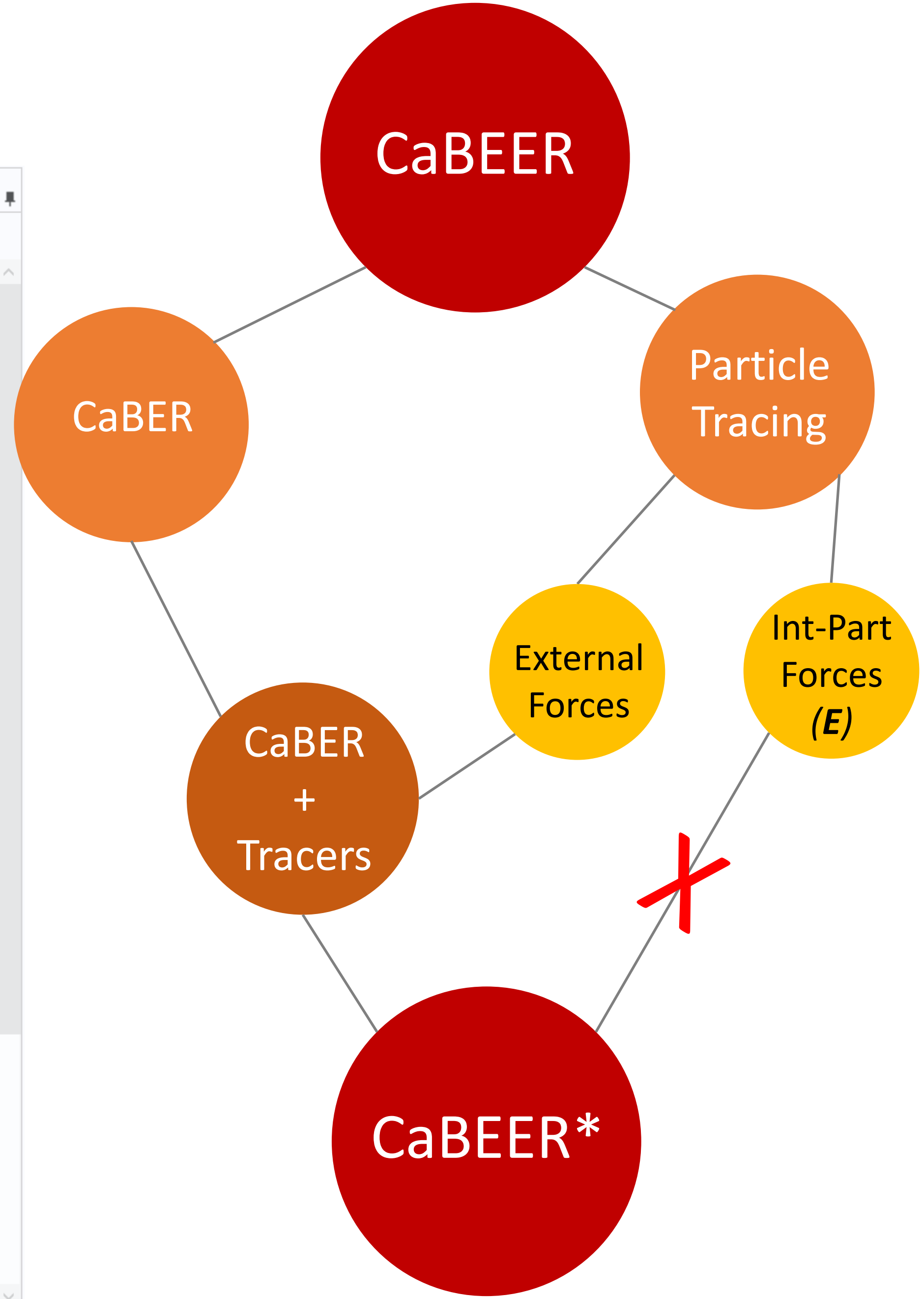
Particle Tracing for Fluid Flow – Interparticle force



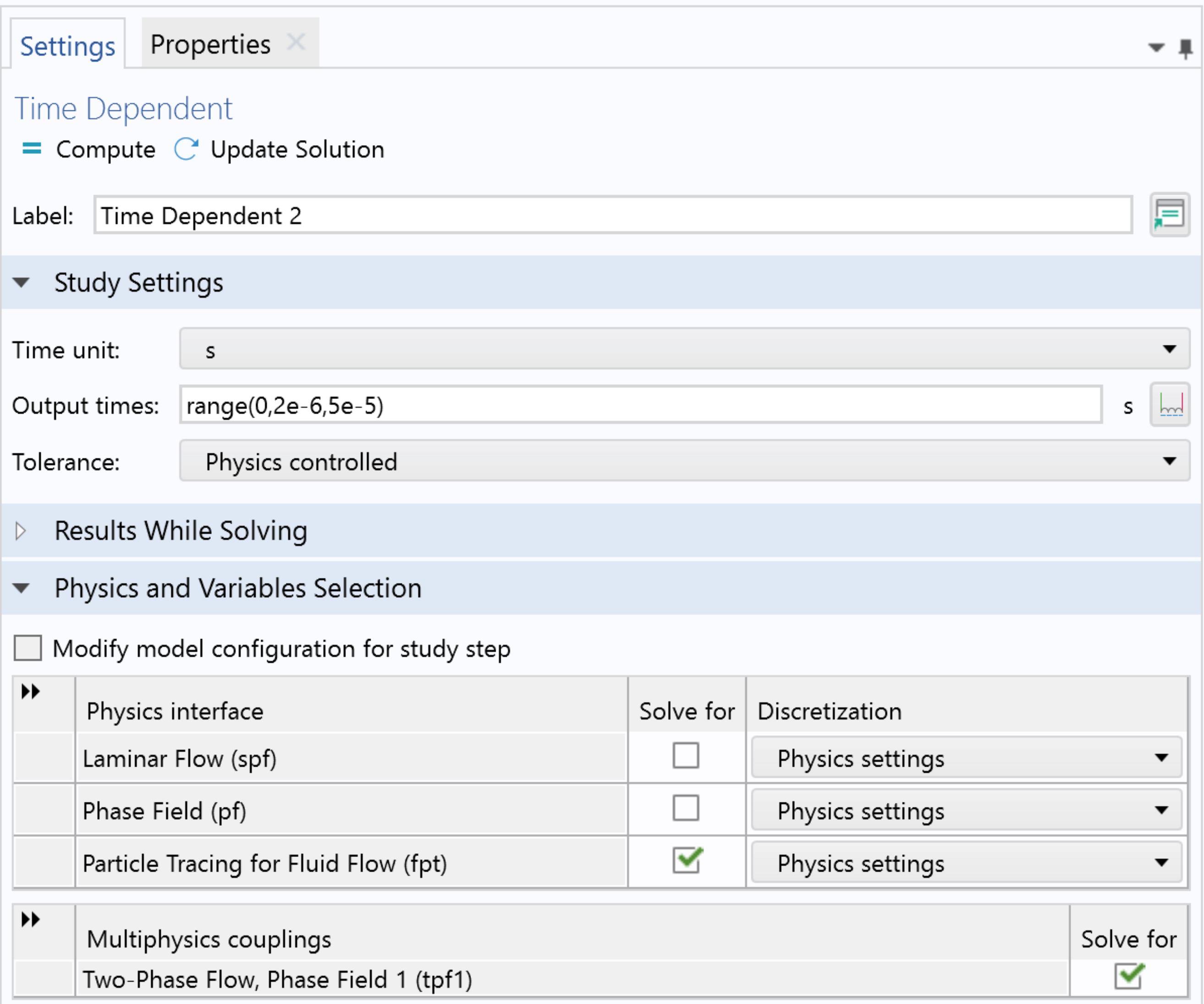


CaBEER*.mph


Model Builder
CaBEER.mph (root)
Global Definitions
Parameters 1
Default Model Inputs
Materials
Component 1 (comp1)
Definitions
Geometry 1
Materials
Laminar Flow (spf)
Phase Field (pf)
Particle Tracing for Fluid Flow (fpt)
Axial Symmetry 1
Wall 1
Particle Properties 1
Outlet 1
Drag Force 1
Release from Grid 1
Brownian Force 1
Gravity Force 1
Multiphysics
Meshes
Study 1
Parametric Sweep
Step 1: Phase Initialization
Step 2: Time Dependent
Step 3: Time Dependent 2
Solver Configurations
Results
Settings
Properties
Drag Force
Label: Drag Force 1
Domain Selection
Selection: Manual
1
Override and Contribution
Equation
Model Input
Coordinate System Selection
Coordinate system:
Global coordinate system
Drag Force
Drag law:
Stokes
Velocity:
u Velocity field (spf)
Dynamic viscosity:
μ From material
Density:
ρ From material
Wall Corrections
Include wall corrections

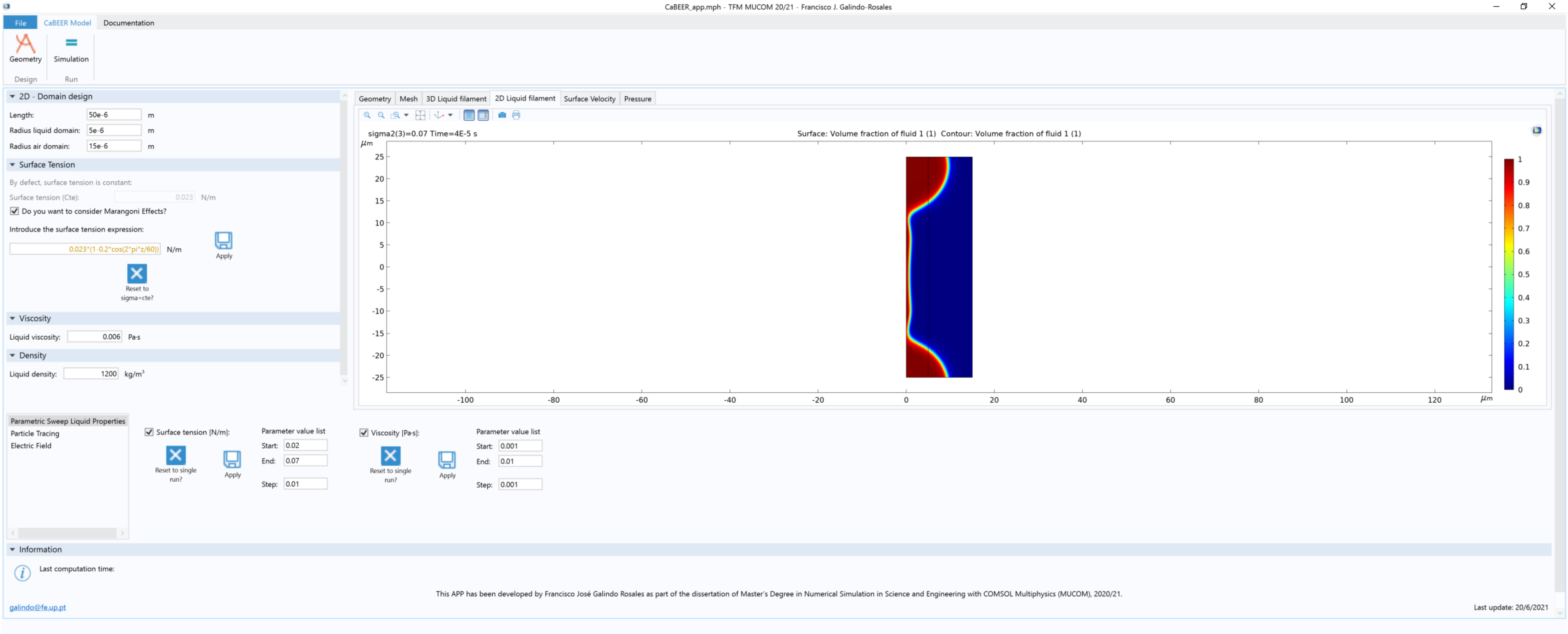

CaBEER
CaBER
Particle Tracing
External Forces
Int-Part Forces (E)
CaBER + Tracers
CaBEER*

CaBEER*.mph


Settings
Properties
Time Dependent
Compute
Update Solution
Label: Time Dependent 2
Study Settings
Time unit: s
Output times: range(0,2e-6,5e-5) s
Tolerance: Physics controlled
Results While Solving
Physics and Variables Selection
Modify model configuration for study step
Physics interface
Solve for
Discretization
Laminar Flow (spf)
Physics settings
Phase Field (pf)
Physics settings
Particle Tracing for Fluid Flow (fpt)
Physics settings
Multiphysics couplings
Solve for
Two-Phase Flow, Phase Field 1 (tpf1)

Implementation

CaBEER-APP



Remarks

- CaBEERTwoPhaseFlow.mph: implemented and working
- ParticleTracing.mph: implemented and working only for external forces
- CaBEER.mph: Implemented and working with no particle-fluid interaction
- CaBEER-APP: Implemented and working for CaBEERTwoPhaseFlow.mph

Future works

- Incorporate the inter-particle force due to the electric field
- Complete the CaBEER-APP
- Run numerical experiments and assess them with experimental results

Acknoledgements

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UNIÃO EUROPEIA
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PORTUGAL 2020
COMPETE 2020
NORTE 2020
REPÚBLICA PORTUGUESA
FCT Fundação para a Ciência e a Tecnologia

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Supervisor: Emilio Ruiz Reina

25 de Junio de 2021

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COMSOL

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