



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

Author: Francisco José Galindo Rosales

Supervisor: Emilio Ruiz Reina

25 de Junio de 2021



UNIVERSIDAD
DE MÁLAGA



uma.es

Content

- Introduction
- Capillary Breakup Extensional Electrorheometry (CaBEER)
- Modelling
- Implementation
- Remarks & Future works

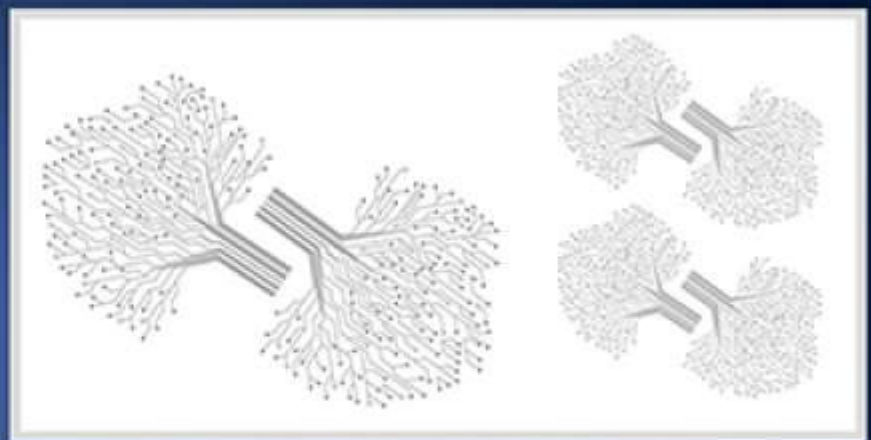


Printer



Material

PRINTED ELECTRONICS MARKET



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.

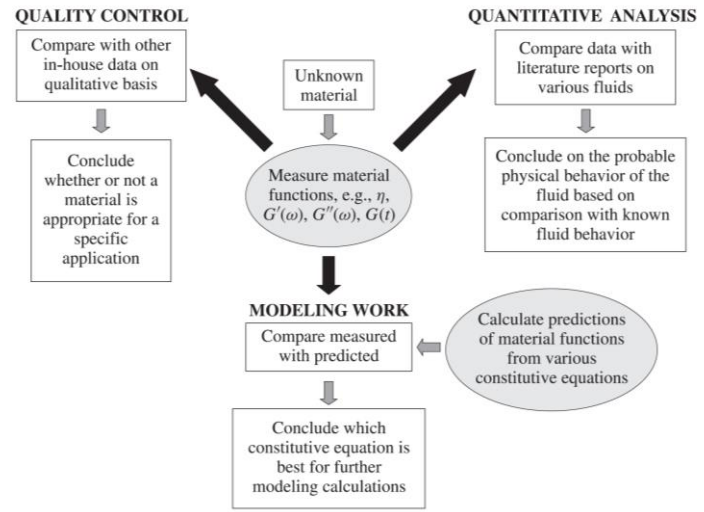
\$363.1 BILLION ← 2030

\$35.7 BILLION ← 2019

CAGR 22.4%
(2020–2030)



© OE-A 2009



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)

Printing

Rheology



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



Chemistry

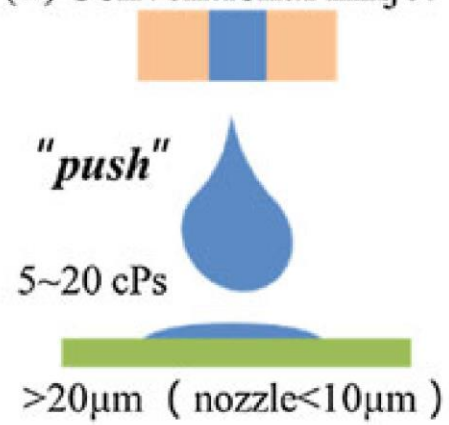


Microelectronics

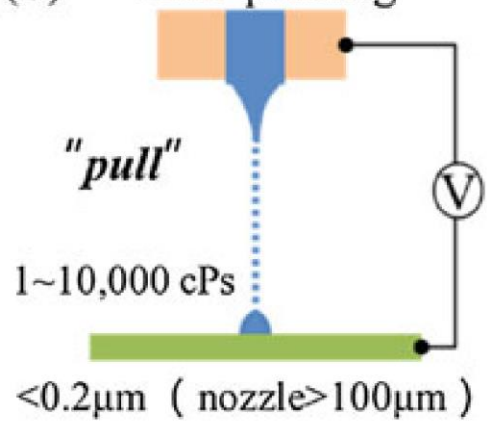
Organic and Printed Electronics

Source: Heraeus, manroland, Infineon, Karl Knauer

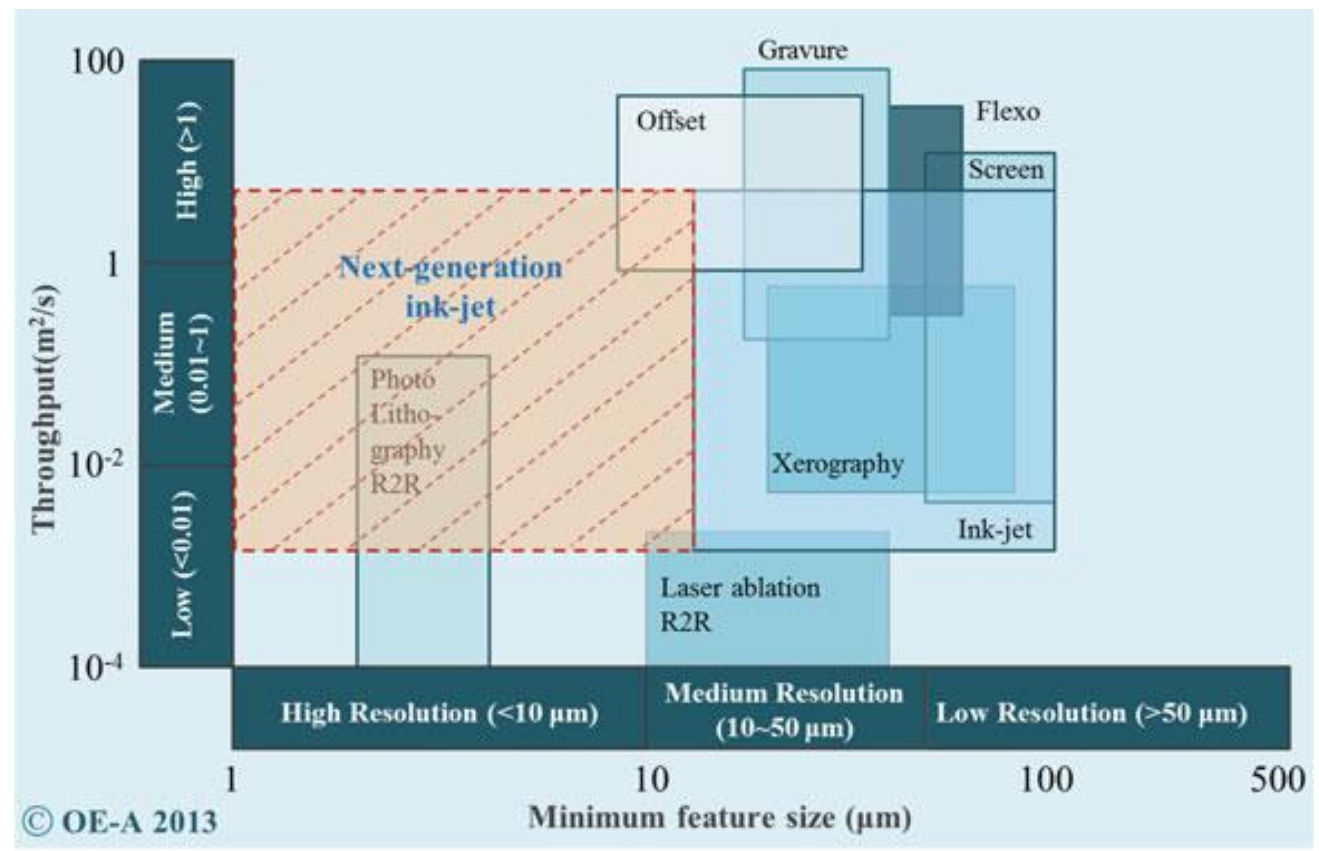
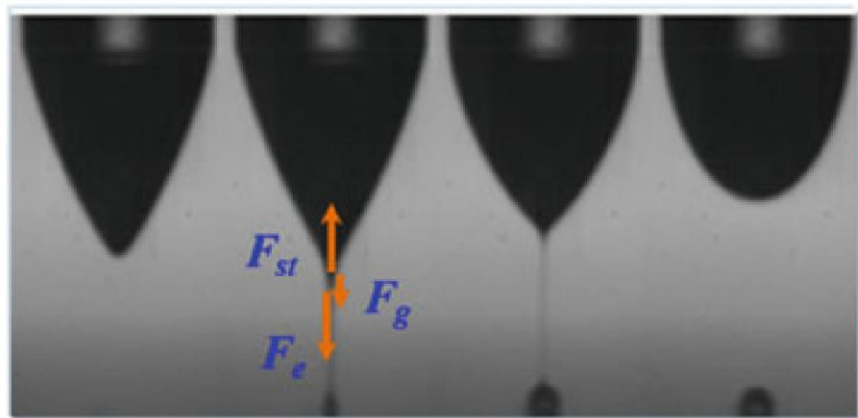
(a) Conventional inkjet

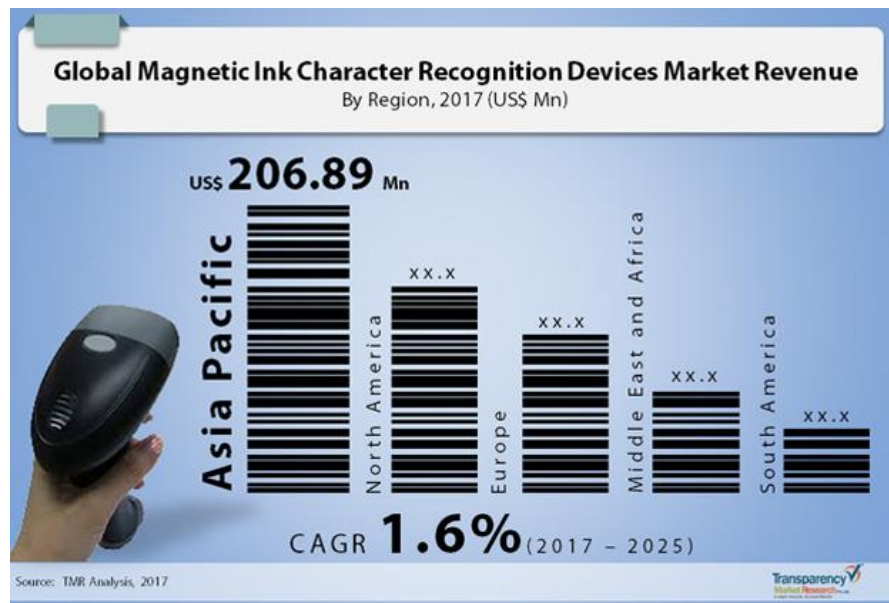


(b) EHD printing



(c)



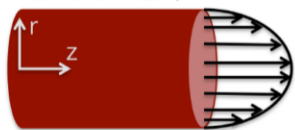


COMSOL model for the Capillary Breakup Extensional Electrorheometry (CaBEER) applied to functional inks

Macro-scale Rheometry

Shear rheometry

Capillary flow

$$\tau_R = (P_0 - P_L)R/2L$$


$$\dot{\gamma}_R = \frac{4Q}{\pi R^3}$$

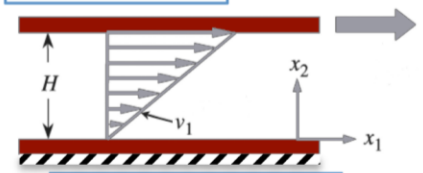
$$\mu = \frac{(P_0 - P_L)R}{2L} \left(\frac{\pi R^3}{4Q} \right)^{-1}$$

$$\dot{\gamma}_R = \dot{\gamma}_0 \left[\frac{1}{4} \left(3 + \frac{d \ln \dot{\gamma}_0}{d \ln \tau_R} \right) \right]$$

$$\eta(\dot{\gamma}_R) = \frac{4\tau_R}{\dot{\gamma}_0} \left(3 + \frac{d \ln \dot{\gamma}_0}{d \ln \tau_R} \right)^{-1}$$

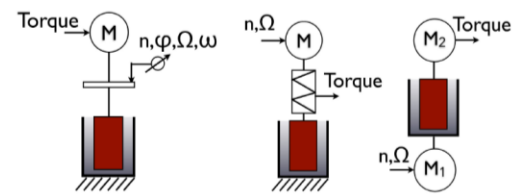
Capillary rheometers

Drag flow

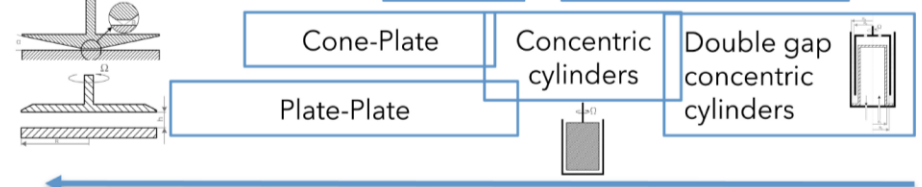


Rotational rheometers

Control Stress Control Strain



Searle Searle / Couette

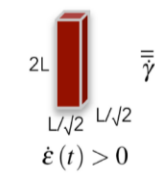


$\eta \uparrow$

Extensional rheometry



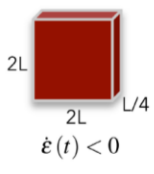
Uniaxial extensional flow



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

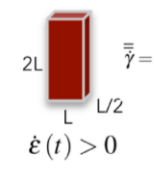
$\dot{\epsilon}(t) > 0$

Biaxial stretching flow



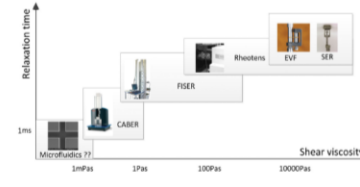
$\dot{\epsilon}(t) < 0$

Planar elongational flow



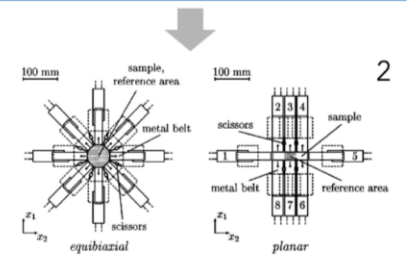
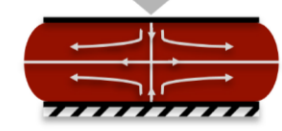
$$\bar{\dot{\gamma}} = \begin{pmatrix} -2\dot{\epsilon}(t) & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 2\dot{\epsilon}(t) \end{pmatrix}$$

$\dot{\epsilon}(t) > 0$



1 Squeeze flow in rotational rheometers

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

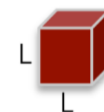


F.J. Galindo-Rosales.
 "Complex fluids and Rheometry in microfluidics".
 Chapter 1 in Complex fluid-flows in microfluidics,
 Springer International Publishing (2018).

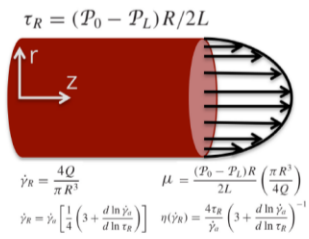
Macro-scale Rheometry

Shear rheometry

Extensional rheometry

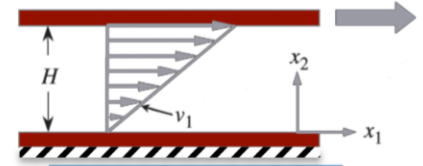


Capillary flow



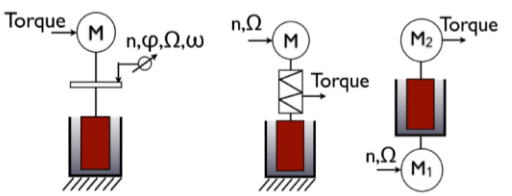
Capillary rheometers

Drag flow

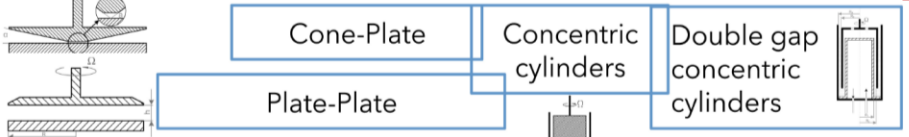


Rotational rheometers

Control Stress Control Strain

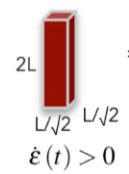


Searle Searle / Couette



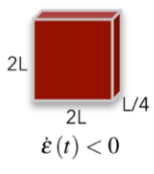
$\eta \uparrow$

Uniaxial extensional flow

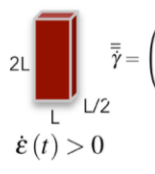


$$\bar{\dot{\gamma}} = \begin{pmatrix} -\dot{\epsilon}(t) & 0 & 0 \\ 0 & -\dot{\epsilon}(t) & 0 \\ 0 & 0 & 2\dot{\epsilon}(t) \end{pmatrix}$$

Biaxial stretching flow



Planar elongational flow

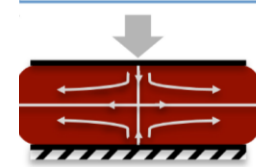


$$\bar{\dot{\gamma}} = \begin{pmatrix} -2\dot{\epsilon}(t) & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 2\dot{\epsilon}(t) \end{pmatrix}$$

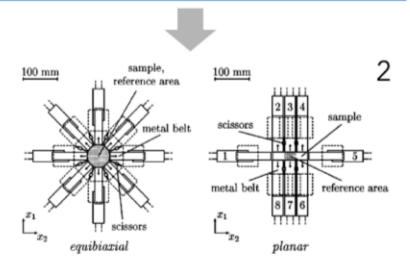


CaBER-1
Thermo Scientific

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).



ELECTRIC FIELD

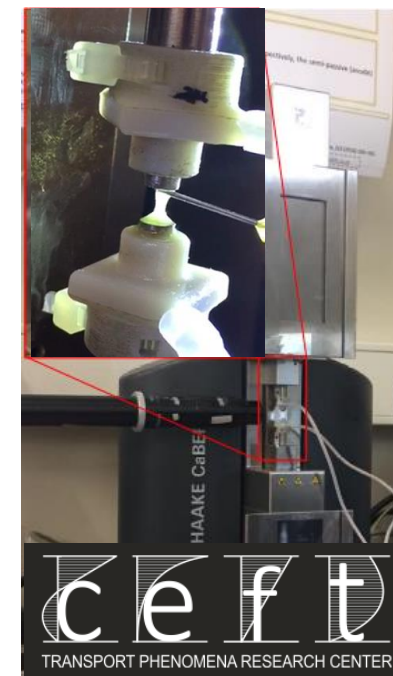
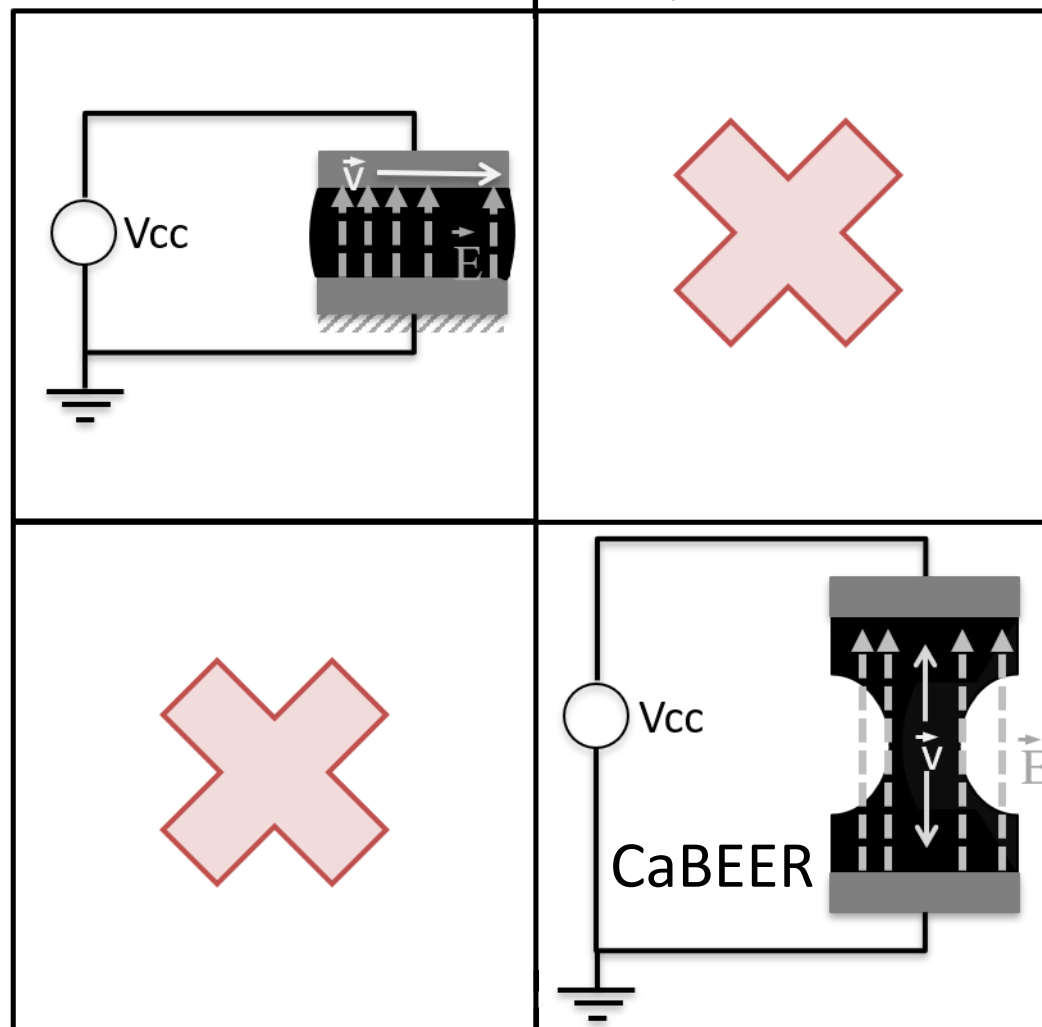
PERPENDICULAR

PARALLEL

FLOW FIELD

SHEAR

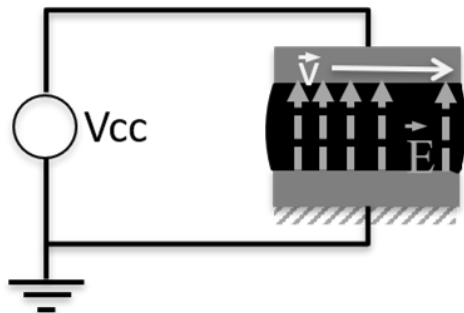
EXTENSIONAL



(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)
 (10) International Publication Number WO 2020/208550 A1



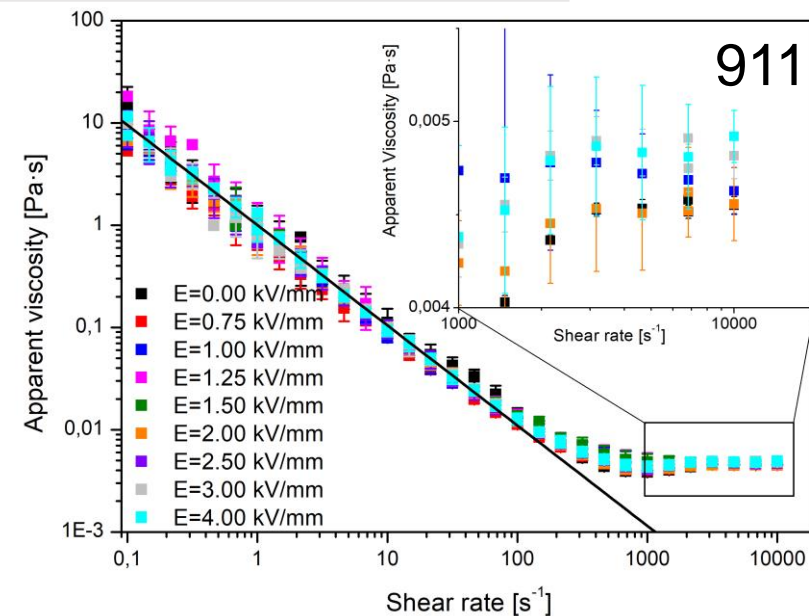
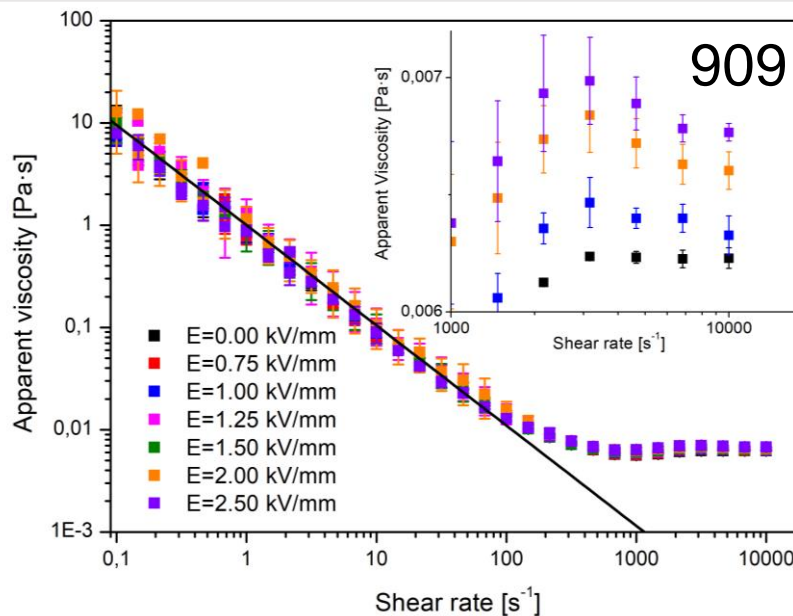
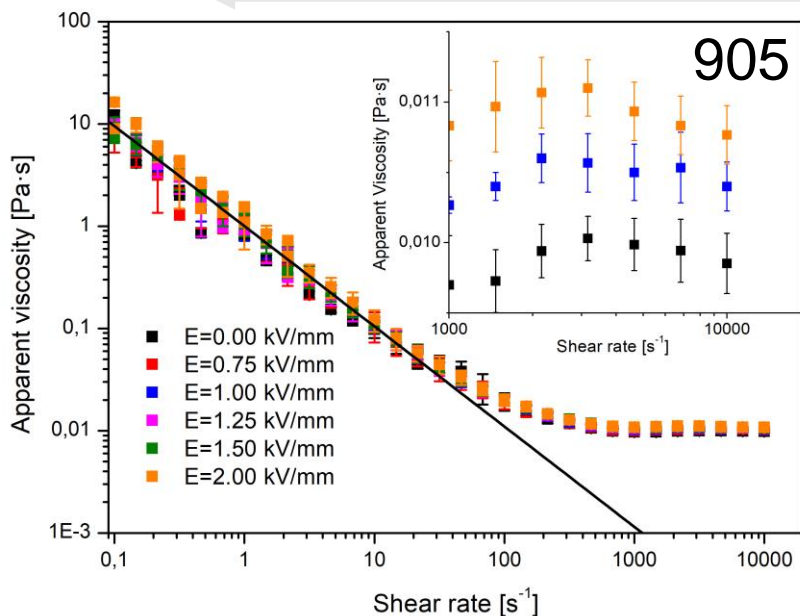
EMG Oil-based Ferrofluid



	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
M_s (mT)	44	22	11
χ	3.52	1.38	0.50
ϕ (% vol)	7.8	3.9	2

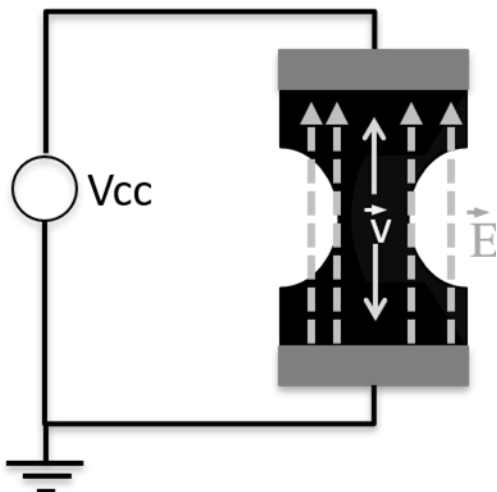
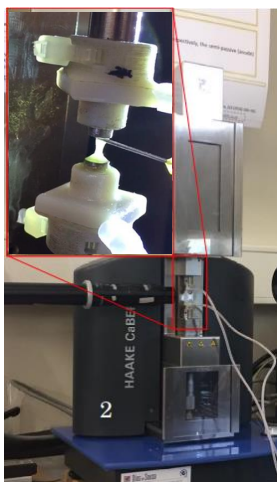
J.H. García-Ortiz and F.J. Galindo-Rosales, JOR (2021) – In preparation
 J.H. García-Ortiz and F.J. Galindo-Rosales, IRC (2020)

ϕ (%vol)



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

EMG Oil-based Ferrofluid



CaBEER

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

Image post-processing

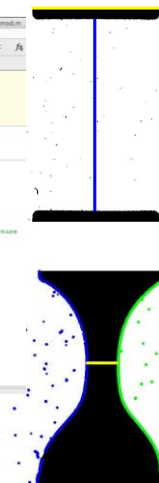
```

1  % This version on 24/2/2019 for the analysis of the
2  % and response of images recorded in the CaBEER device.
3  % This Matlab file should be located in the folder containing the set of
4  % images to be analyzed.
5  % The file will be reported: 1) containing the line evolution of the
6  % minimum diameter (in mm and normalized) and the vertical position. 2) the
7  % diameter
8  %
9  %
10 %
11 %
12 %
13 %
14 %
15 %
16 %
17 %
18 %
19 %
20 %
21 %
22 %
23 %
24 %
25 %
26 %
27 %
28 %
29 %
30 %
31 %
32 %
33 %
34 %
35 %
36 %
37 %
38 %
39 %
40 %
41 %
42 %
43 %
44 %
45 %
46 %
47 %
48 %
49 %
50 %
51 %
52 %
53 %
54 %
55 %
56 %
57 %
58 %
59 %
60 %
61 %
62 %
63 %
64 %
65 %
66 %
67 %
68 %
69 %
70 %
71 %
72 %
73 %
74 %
75 %
76 %
77 %
78 %
79 %
80 %
81 %
82 %
83 %
84 %
85 %
86 %
87 %
88 %
89 %
90 %
91 %
92 %
93 %
94 %
95 %
96 %
97 %
98 %
99 %
100 %
101 %
102 %
103 %
104 %
105 %
106 %
107 %
108 %
109 %
110 %
111 %
112 %
113 %
114 %
115 %
116 %
117 %
118 %
119 %
120 %
121 %
122 %
123 %
124 %
125 %
126 %
127 %
128 %
129 %
130 %
131 %
132 %
133 %
134 %
135 %
136 %
137 %
138 %
139 %
140 %
141 %
142 %
143 %
144 %
145 %
146 %
147 %
148 %
149 %
150 %
151 %
152 %
153 %
154 %
155 %
156 %
157 %
158 %
159 %
160 %
161 %
162 %
163 %
164 %
165 %
166 %
167 %
168 %
169 %
170 %
171 %
172 %
173 %
174 %
175 %
176 %
177 %
178 %
179 %
180 %
181 %
182 %
183 %
184 %
185 %
186 %
187 %
188 %
189 %
190 %
191 %
192 %
193 %
194 %
195 %
196 %
197 %
198 %
199 %
200 %
201 %
202 %
203 %
204 %
205 %
206 %
207 %
208 %
209 %
210 %
211 %
212 %
213 %
214 %
215 %
216 %
217 %
218 %
219 %
220 %
221 %
222 %
223 %
224 %
225 %
226 %
227 %
228 %
229 %
230 %
231 %
232 %
233 %
234 %
235 %
236 %
237 %
238 %
239 %
240 %
241 %
242 %
243 %
244 %
245 %
246 %
247 %
248 %
249 %
250 %
251 %
252 %
253 %
254 %
255 %
256 %
257 %
258 %
259 %
260 %
261 %
262 %
263 %
264 %
265 %
266 %
267 %
268 %
269 %
270 %
271 %
272 %
273 %
274 %
275 %
276 %
277 %
278 %
279 %
280 %
281 %
282 %
283 %
284 %
285 %
286 %
287 %
288 %
289 %
290 %
291 %
292 %
293 %
294 %
295 %
296 %
297 %
298 %
299 %
300 %
301 %
302 %
303 %
304 %
305 %
306 %
307 %
308 %
309 %
310 %
311 %
312 %
313 %
314 %
315 %
316 %
317 %
318 %
319 %
320 %
321 %
322 %
323 %
324 %
325 %
326 %
327 %
328 %
329 %
330 %
331 %
332 %
333 %
334 %
335 %
336 %
337 %
338 %
339 %
340 %
341 %
342 %
343 %
344 %
345 %
346 %
347 %
348 %
349 %
350 %
351 %
352 %
353 %
354 %
355 %
356 %
357 %
358 %
359 %
360 %
361 %
362 %
363 %
364 %
365 %
366 %
367 %
368 %
369 %
370 %
371 %
372 %
373 %
374 %
375 %
376 %
377 %
378 %
379 %
380 %
381 %
382 %
383 %
384 %
385 %
386 %
387 %
388 %
389 %
390 %
391 %
392 %
393 %
394 %
395 %
396 %
397 %
398 %
399 %
400 %
401 %
402 %
403 %
404 %
405 %
406 %
407 %
408 %
409 %
410 %
411 %
412 %
413 %
414 %
415 %
416 %
417 %
418 %
419 %
420 %
421 %
422 %
423 %
424 %
425 %
426 %
427 %
428 %
429 %
430 %
431 %
432 %
433 %
434 %
435 %
436 %
437 %
438 %
439 %
440 %
441 %
442 %
443 %
444 %
445 %
446 %
447 %
448 %
449 %
450 %
451 %
452 %
453 %
454 %
455 %
456 %
457 %
458 %
459 %
460 %
461 %
462 %
463 %
464 %
465 %
466 %
467 %
468 %
469 %
470 %
471 %
472 %
473 %
474 %
475 %
476 %
477 %
478 %
479 %
480 %
481 %
482 %
483 %
484 %
485 %
486 %
487 %
488 %
489 %
490 %
491 %
492 %
493 %
494 %
495 %
496 %
497 %
498 %
499 %
500 %
501 %
502 %
503 %
504 %
505 %
506 %
507 %
508 %
509 %
510 %
511 %
512 %
513 %
514 %
515 %
516 %
517 %
518 %
519 %
520 %
521 %
522 %
523 %
524 %
525 %
526 %
527 %
528 %
529 %
530 %
531 %
532 %
533 %
534 %
535 %
536 %
537 %
538 %
539 %
540 %
541 %
542 %
543 %
544 %
545 %
546 %
547 %
548 %
549 %
550 %
551 %
552 %
553 %
554 %
555 %
556 %
557 %
558 %
559 %
560 %
561 %
562 %
563 %
564 %
565 %
566 %
567 %
568 %
569 %
570 %
571 %
572 %
573 %
574 %
575 %
576 %
577 %
578 %
579 %
580 %
581 %
582 %
583 %
584 %
585 %
586 %
587 %
588 %
589 %
590 %
591 %
592 %
593 %
594 %
595 %
596 %
597 %
598 %
599 %
600 %
601 %
602 %
603 %
604 %
605 %
606 %
607 %
608 %
609 %
610 %
611 %
612 %
613 %
614 %
615 %
616 %
617 %
618 %
619 %
620 %
621 %
622 %
623 %
624 %
625 %
626 %
627 %
628 %
629 %
630 %
631 %
632 %
633 %
634 %
635 %
636 %
637 %
638 %
639 %
640 %
641 %
642 %
643 %
644 %
645 %
646 %
647 %
648 %
649 %
650 %
651 %
652 %
653 %
654 %
655 %
656 %
657 %
658 %
659 %
660 %
661 %
662 %
663 %
664 %
665 %
666 %
667 %
668 %
669 %
670 %
671 %
672 %
673 %
674 %
675 %
676 %
677 %
678 %
679 %
680 %
681 %
682 %
683 %
684 %
685 %
686 %
687 %
688 %
689 %
690 %
691 %
692 %
693 %
694 %
695 %
696 %
697 %
698 %
699 %
700 %
701 %
702 %
703 %
704 %
705 %
706 %
707 %
708 %
709 %
710 %
711 %
712 %
713 %
714 %
715 %
716 %
717 %
718 %
719 %
720 %
721 %
722 %
723 %
724 %
725 %
726 %
727 %
728 %
729 %
730 %
731 %
732 %
733 %
734 %
735 %
736 %
737 %
738 %
739 %
740 %
741 %
742 %
743 %
744 %
745 %
746 %
747 %
748 %
749 %
750 %
751 %
752 %
753 %
754 %
755 %
756 %
757 %
758 %
759 %
760 %
761 %
762 %
763 %
764 %
765 %
766 %
767 %
768 %
769 %
770 %
771 %
772 %
773 %
774 %
775 %
776 %
777 %
778 %
779 %
780 %
781 %
782 %
783 %
784 %
785 %
786 %
787 %
788 %
789 %
790 %
791 %
792 %
793 %
794 %
795 %
796 %
797 %
798 %
799 %
800 %
801 %
802 %
803 %
804 %
805 %
806 %
807 %
808 %
809 %
810 %
811 %
812 %
813 %
814 %
815 %
816 %
817 %
818 %
819 %
820 %
821 %
822 %
823 %
824 %
825 %
826 %
827 %
828 %
829 %
830 %
831 %
832 %
833 %
834 %
835 %
836 %
837 %
838 %
839 %
840 %
841 %
842 %
843 %
844 %
845 %
846 %
847 %
848 %
849 %
850 %
851 %
852 %
853 %
854 %
855 %
856 %
857 %
858 %
859 %
860 %
861 %
862 %
863 %
864 %
865 %
866 %
867 %
868 %
869 %
870 %
871 %
872 %
873 %
874 %
875 %
876 %
877 %
878 %
879 %
880 %
881 %
882 %
883 %
884 %
885 %
886 %
887 %
888 %
889 %
890 %
891 %
892 %
893 %
894 %
895 %
896 %
897 %
898 %
899 %
900 %
901 %
902 %
903 %
904 %
905 %
906 %
907 %
908 %
909 %
910 %
911 %
912 %
913 %
914 %
915 %
916 %
917 %
918 %
919 %
920 %
921 %
922 %
923 %
924 %
925 %
926 %
927 %
928 %
929 %
930 %
931 %
932 %
933 %
934 %
935 %
936 %
937 %
938 %
939 %
940 %
941 %
942 %
943 %
944 %
945 %
946 %
947 %
948 %
949 %
950 %
951 %
952 %
953 %
954 %
955 %
956 %
957 %
958 %
959 %
960 %
961 %
962 %
963 %
964 %
965 %
966 %
967 %
968 %
969 %
970 %
971 %
972 %
973 %
974 %
975 %
976 %
977 %
978 %
979 %
980 %
981 %
982 %
983 %
984 %
985 %
986 %
987 %
988 %
989 %
990 %
991 %
992 %
993 %
994 %
995 %
996 %
997 %
998 %
999 %
1000 %

```

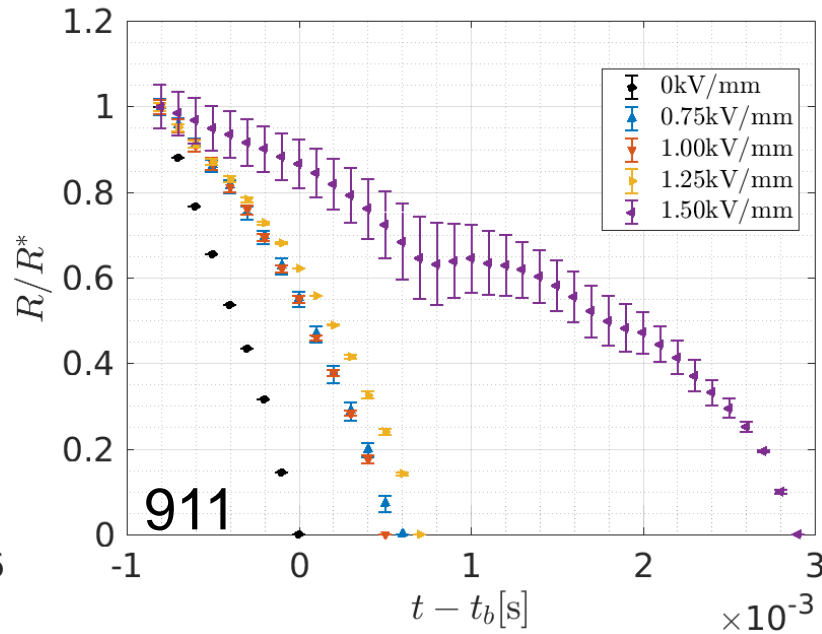
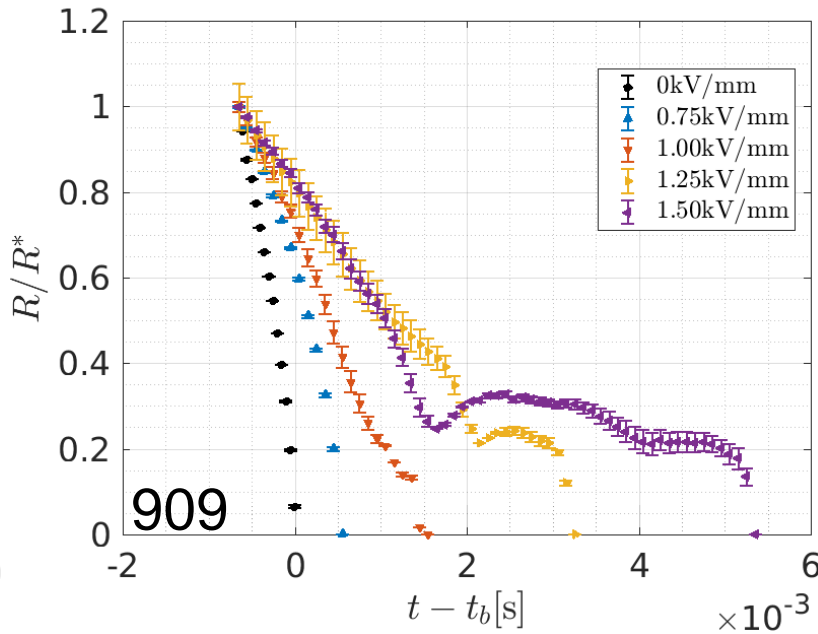
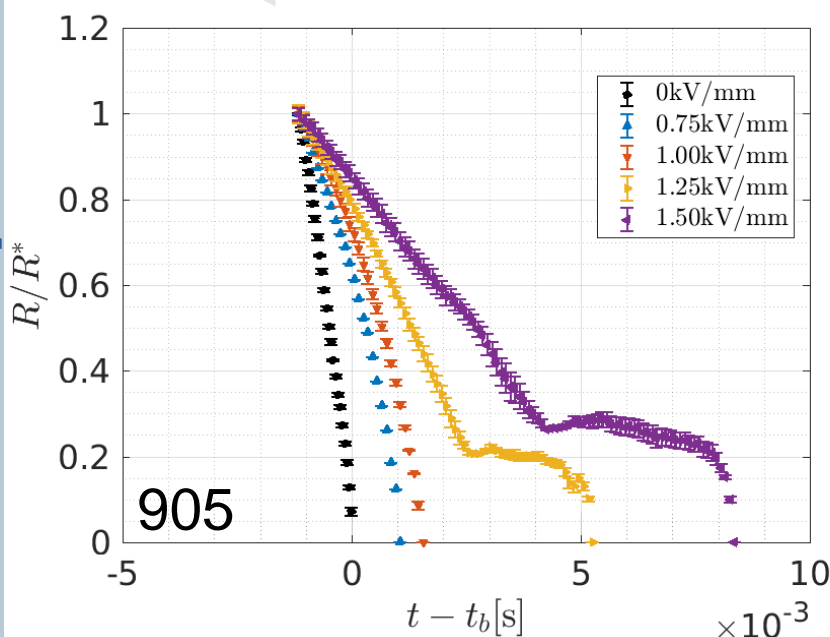


In-house code

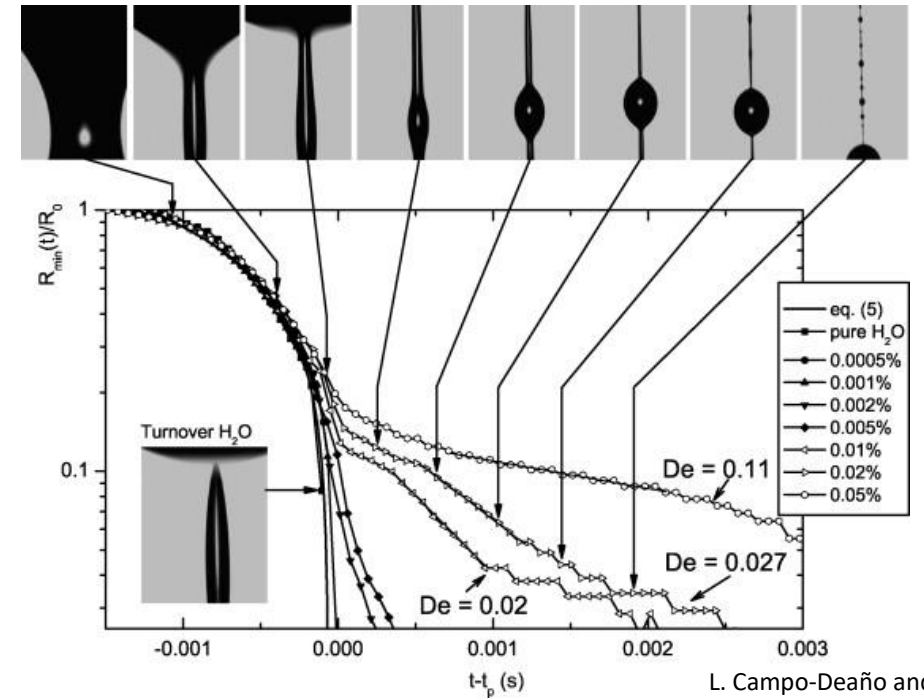
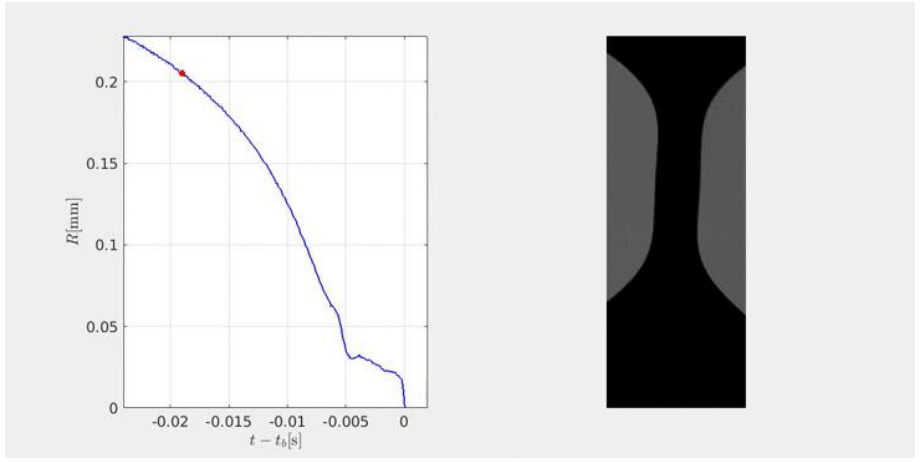


J.H. García-Ortiz and F.J. Galindo-Rosales, JOR (2021) – In preparation
 J.H. García-Ortiz and F.J. Galindo-Rosales, IRC (2020)

ϕ (%vol)



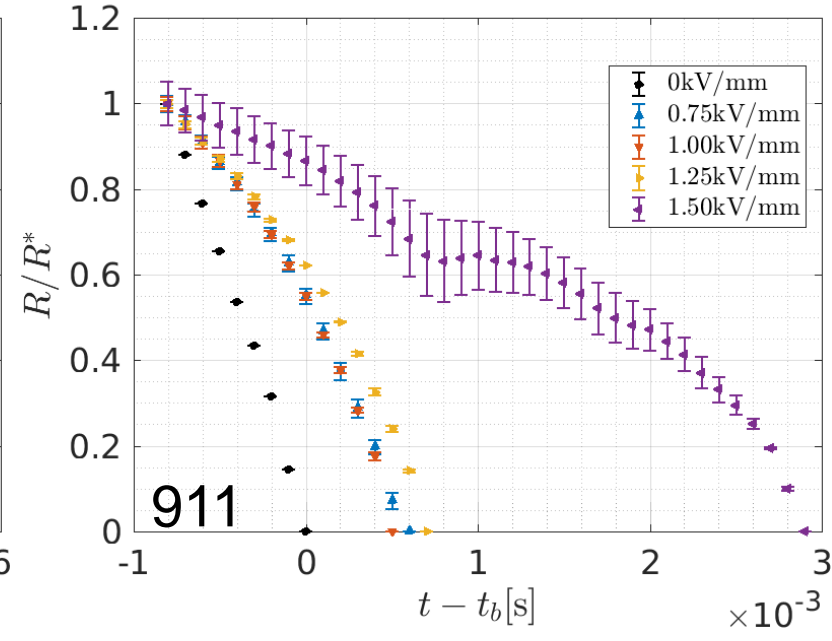
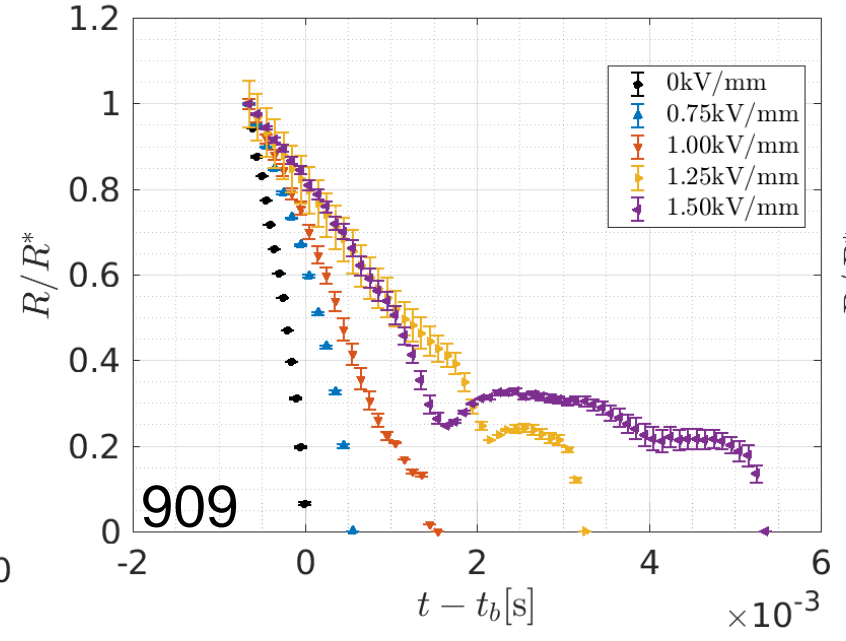
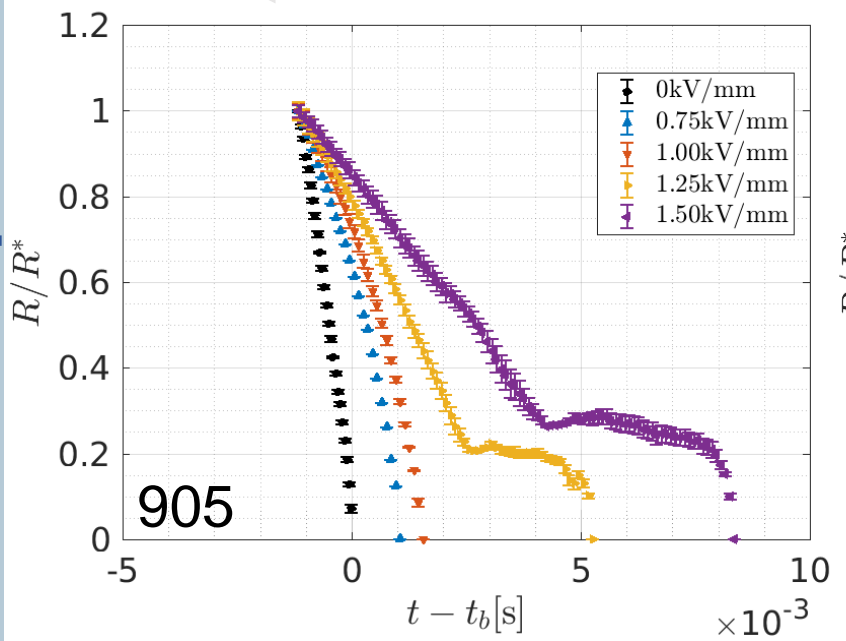
EMG Oil-based Ferrofluid



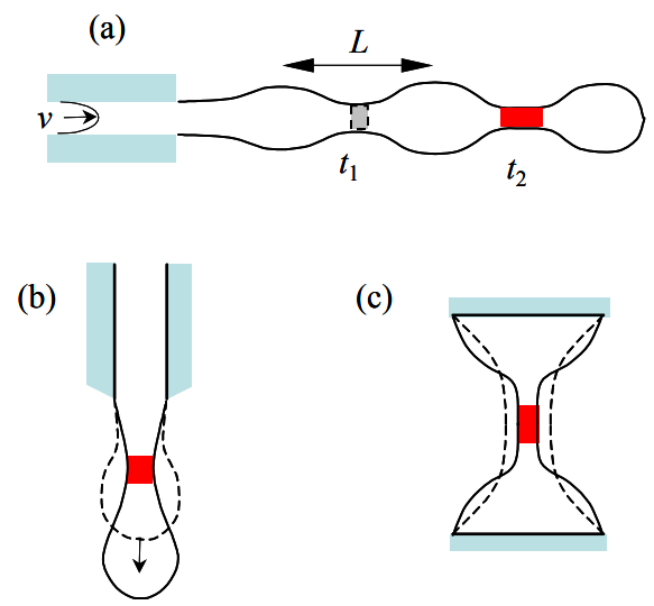
J.H. García-Ortiz and F.J. Galindo-Rosales, JOR (2021) – In preparation
 J.H. García-Ortiz and F.J. Galindo-Rosales, IRC (2020)

ϕ (%vol)

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



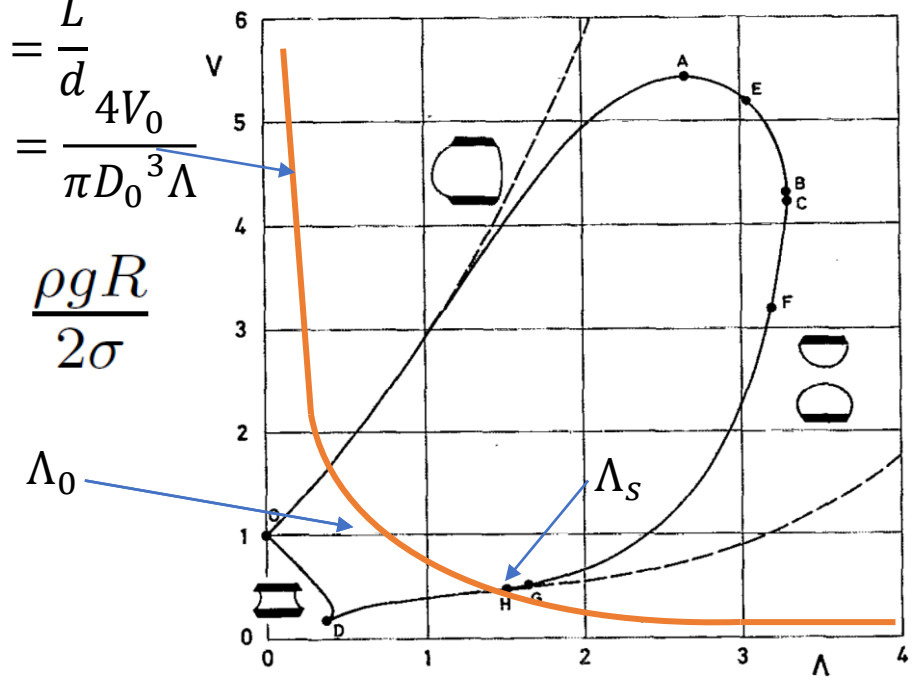
$$Oh = \frac{\mu}{\sqrt{\rho\sigma R}}$$



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

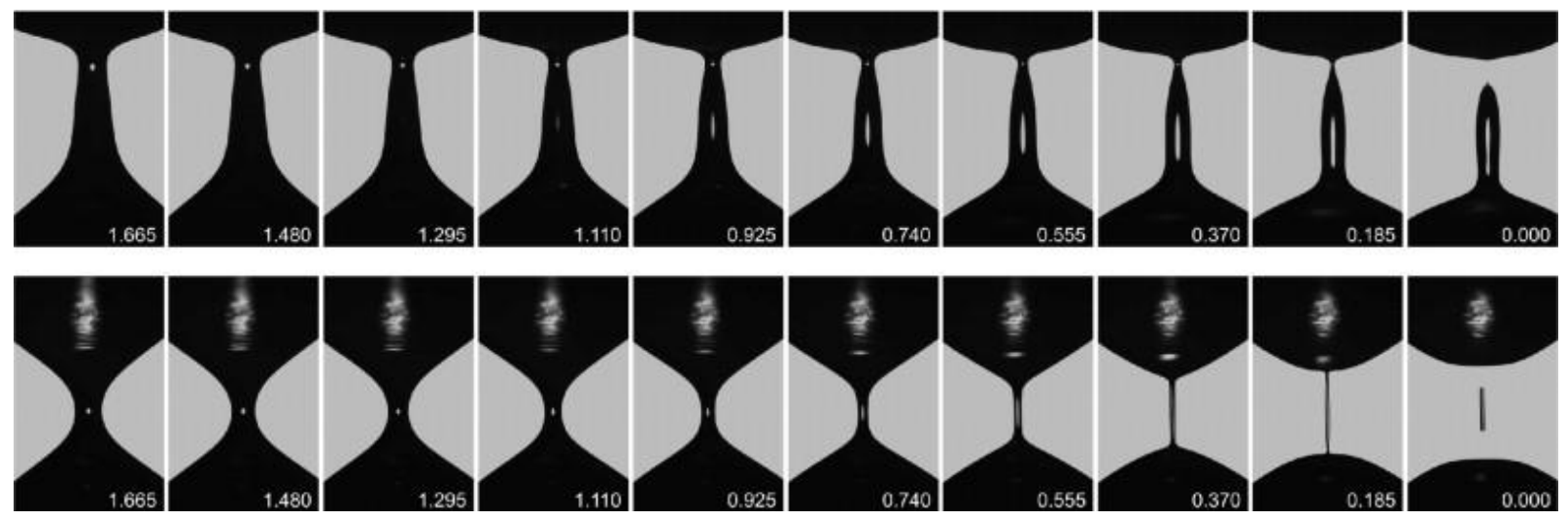
$$V = \frac{4V_0}{\pi D_0^3 \Lambda}$$

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

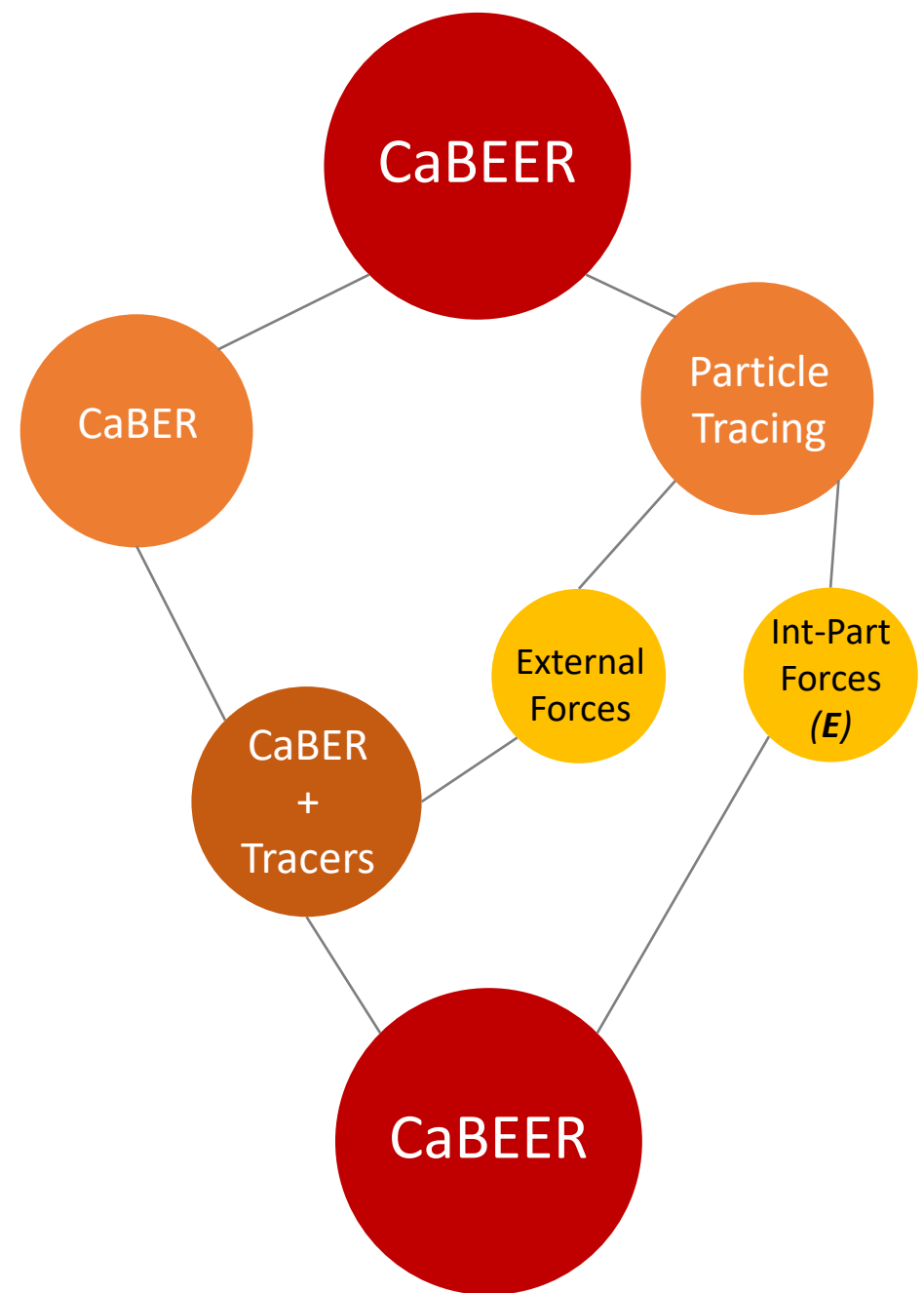
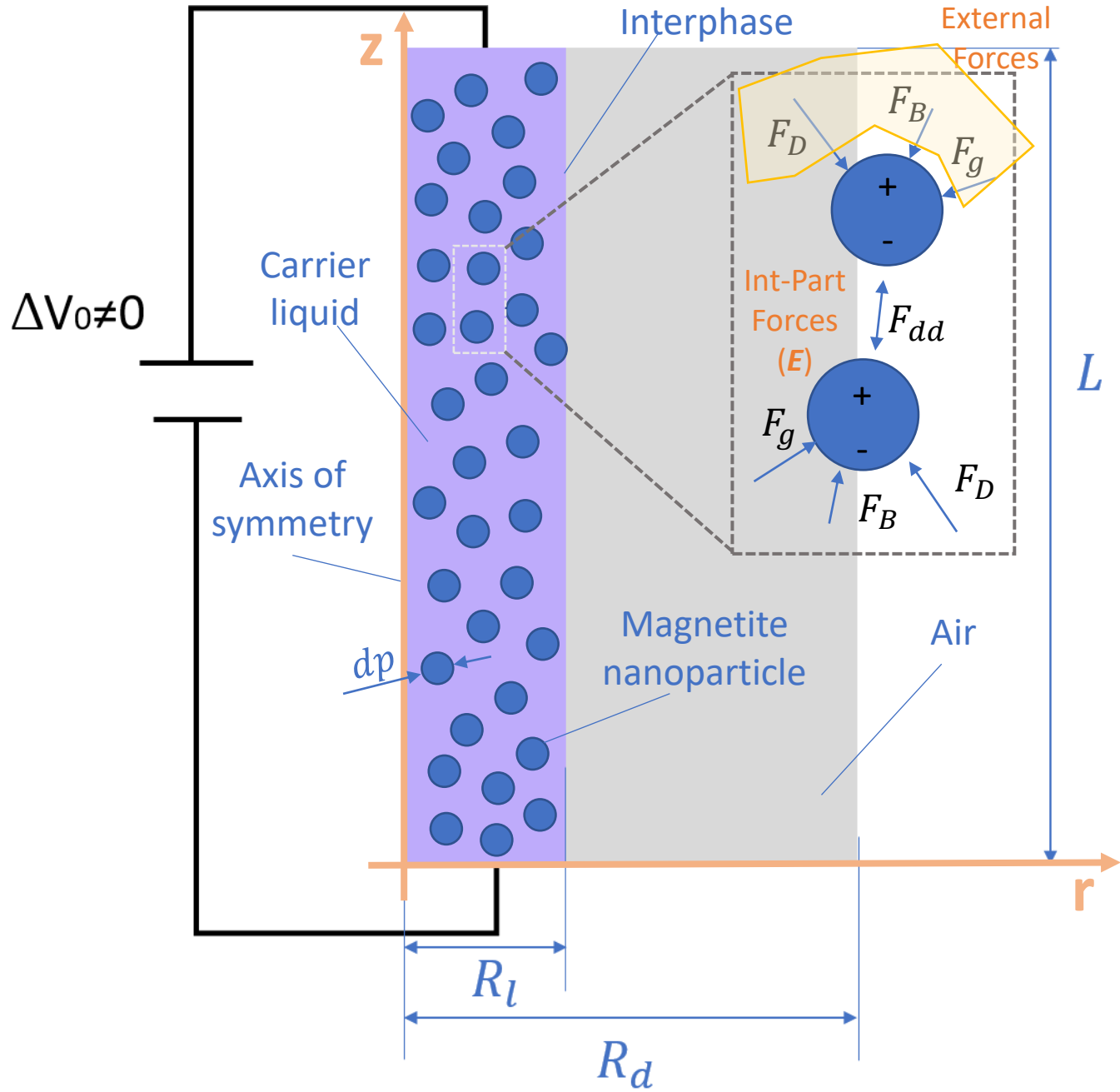


Gareth H. Mckinley. Visco-elasto-capillary thinning and break-up of complex fluids. ANNUAL RHEOLOGY REVIEWS, pages 1–49, 2005.

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.



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

Two Phase Flow, phase field

1. Topology changes are expected.
2. Surface tension effects are important.

Laminar flow

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

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

Phase field method

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

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

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

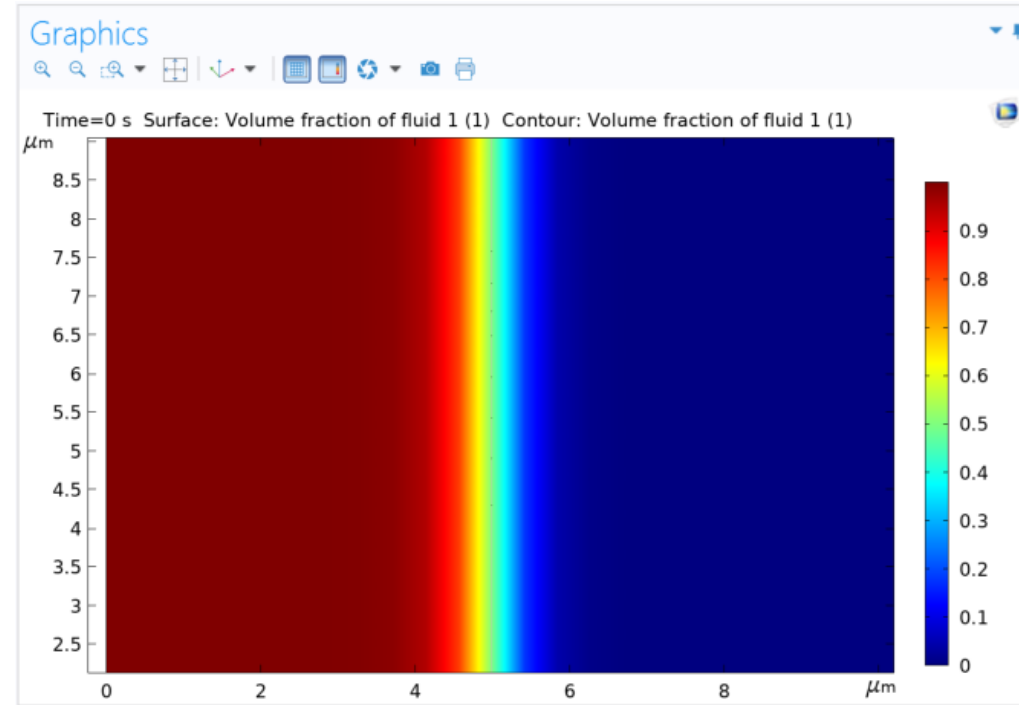
$$\gamma = \chi \epsilon^2,$$

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

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

$$\mathbf{F}_{st} = \left(G - \frac{\partial f}{\partial \Phi} \right) \nabla \Phi$$

$$\left\{ \begin{array}{l} \rho = \rho_l + (\rho_l - \rho_g) V_f \\ \mu = \mu_l + (\mu_l - \mu_g) V_f \\ \epsilon = \epsilon_l + (\epsilon_l - \epsilon_g) V_f \\ \kappa = 2(1 + \Phi)(1 - \Phi) \frac{G}{\sigma} \\ G = \lambda \left(-\nabla^2 \Phi + \frac{\Phi (\Phi^2 - 1)}{\epsilon^2} \right) + \frac{\partial f}{\partial \Phi} \end{array} \right.$$



Two Phase Flow, phase field

Settings Properties

Two-Phase Flow, Phase Field

Label: Two-Phase Flow, Phase Field 1

Name: tpf1

Domain Selection

Selection: All domains

1
2

Equation

Coupled Interfaces

Fluid flow: Laminar Flow (spf)

Moving interface: Phase Field (pf)

Model Input

Temperature: T Common model input

Absolute pressure: pA Absolute pressure (spf)

Settings Properties

Two-Phase Flow, Phase Field

p_A Absolute pressure (spf)

Fluid 1 Properties

Fluid 1: Material 1 (mat1)

Density of fluid 1: ρ_1 From material

Constitutive relation: Newtonian

Dynamic viscosity of fluid 1: μ_1 From material

Fluid 2 Properties

Fluid 2: Material 2 (mat2)

Density of fluid 2: ρ_2 From material

Constitutive relation: Newtonian

Dynamic viscosity of fluid 2: μ_2 From material

Advanced Settings

Surface Tension

Include surface tension force in momentum equation

Include surface tension gradient effects in surface tension force

Surface tension coefficient: User defined

Surface tension coefficient: σ sigma2 N/m

Two Phase Flow, phase field

Settings Properties ×

Phase Initialization

≡ Compute ↻ Update Solution

Label:

▼ Study Settings

▼ Physics and Variables Selection

Modify model configuration for study step

▶▶	Physics interface	Solve for	Discretization
	Laminar Flow (spf)	<input type="checkbox"/>	Physics settings
	Phase Field (pf)	<input checked="" type="checkbox"/>	Physics settings

▶▶	Multiphysics couplings	Solve for
	Two-Phase Flow, Phase Field 1 (tpf1)	<input checked="" type="checkbox"/>

▶ Values of Dependent Variables

▶ Mesh Selection

▶ Adaptation and Error Estimates

▶ Study Extensions

Settings Properties ×

Time Dependent

≡ Compute ↻ Update Solution

Label:

▼ Study Settings

Time unit:

Output times: s

Tolerance:

▶ Results While Solving

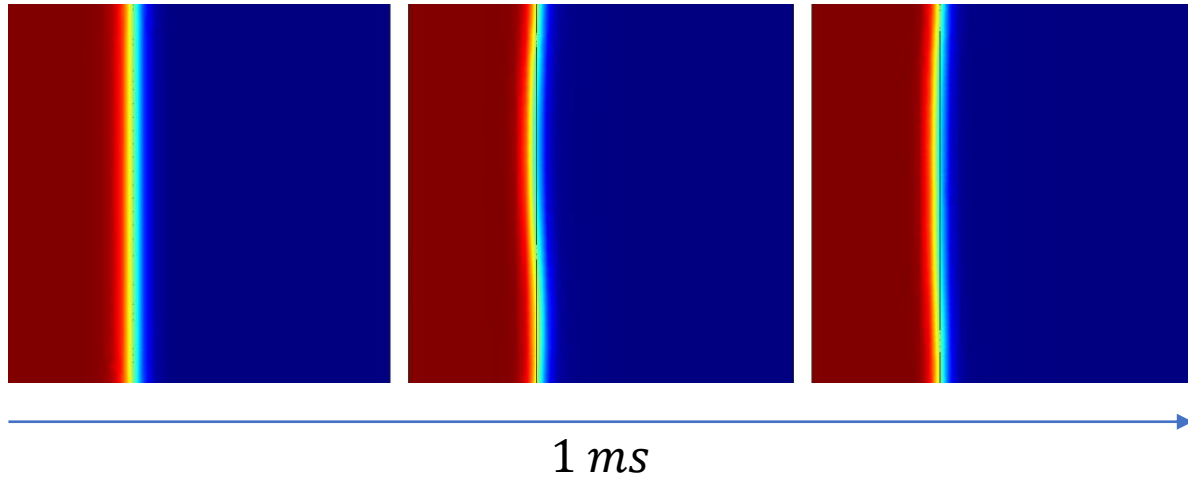
▼ Physics and Variables Selection

Modify model configuration for study step

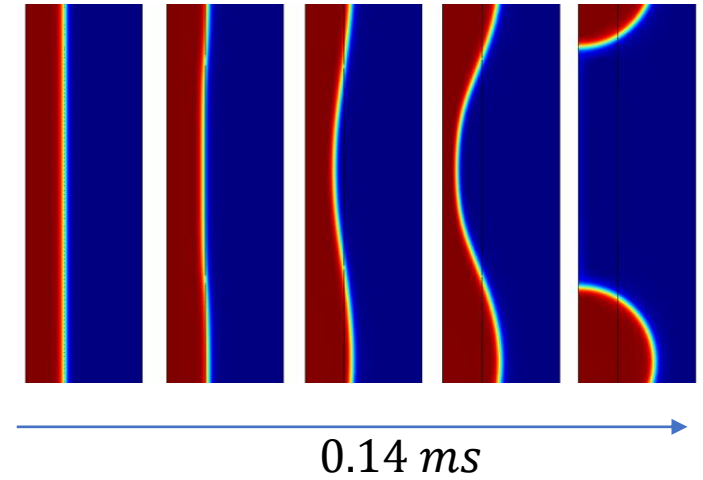
▶▶	Physics interface	Solve for	Discretization
	Laminar Flow (spf)	<input checked="" type="checkbox"/>	Physics settings
	Phase Field (pf)	<input checked="" type="checkbox"/>	Physics settings

▶▶	Multiphysics couplings	Solve for
	Two-Phase Flow, Phase Field 1 (tpf1)	<input checked="" type="checkbox"/>

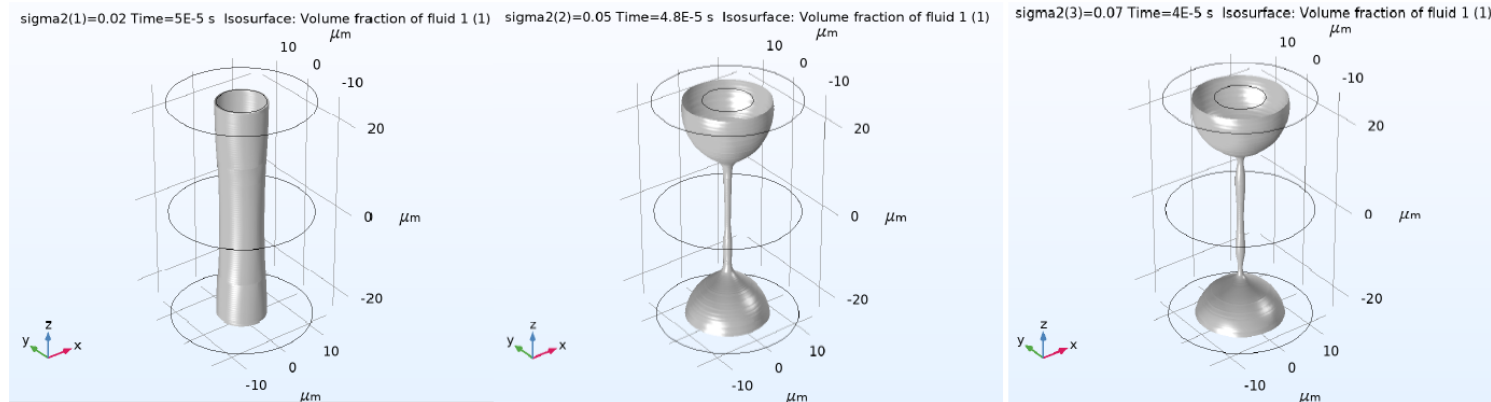
Two Phase Flow, phase field



$$\Lambda_1 = 1.5$$



$$\Lambda_2 = 5$$



(a) $\sigma = 0.02$

(b) $\sigma = 0.05$

(c) $\sigma = 0.07$

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

Particle Tracing for Fluid Flow

External forces

Brownian force (F_B)

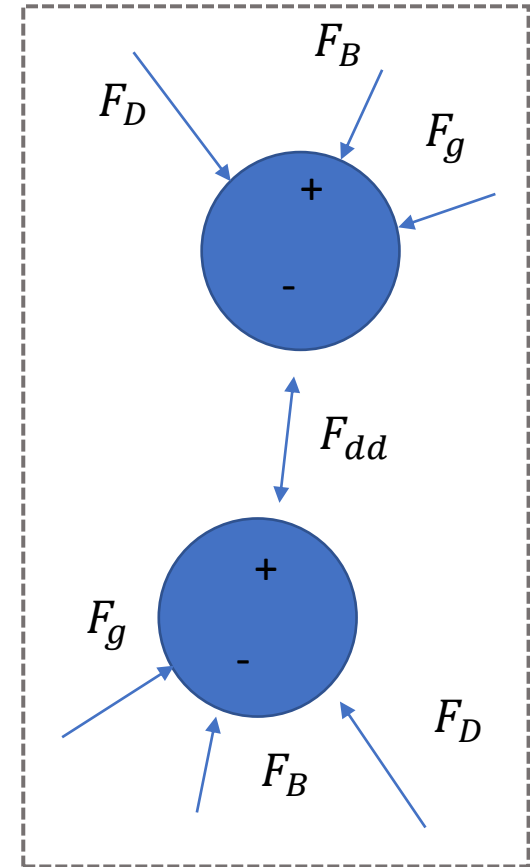
$$F_B = \zeta \sqrt{\frac{6\pi k_B \mu T d_p}{\Delta t}}$$

Drag force (F_D)

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

Gravitational force (F_g)

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

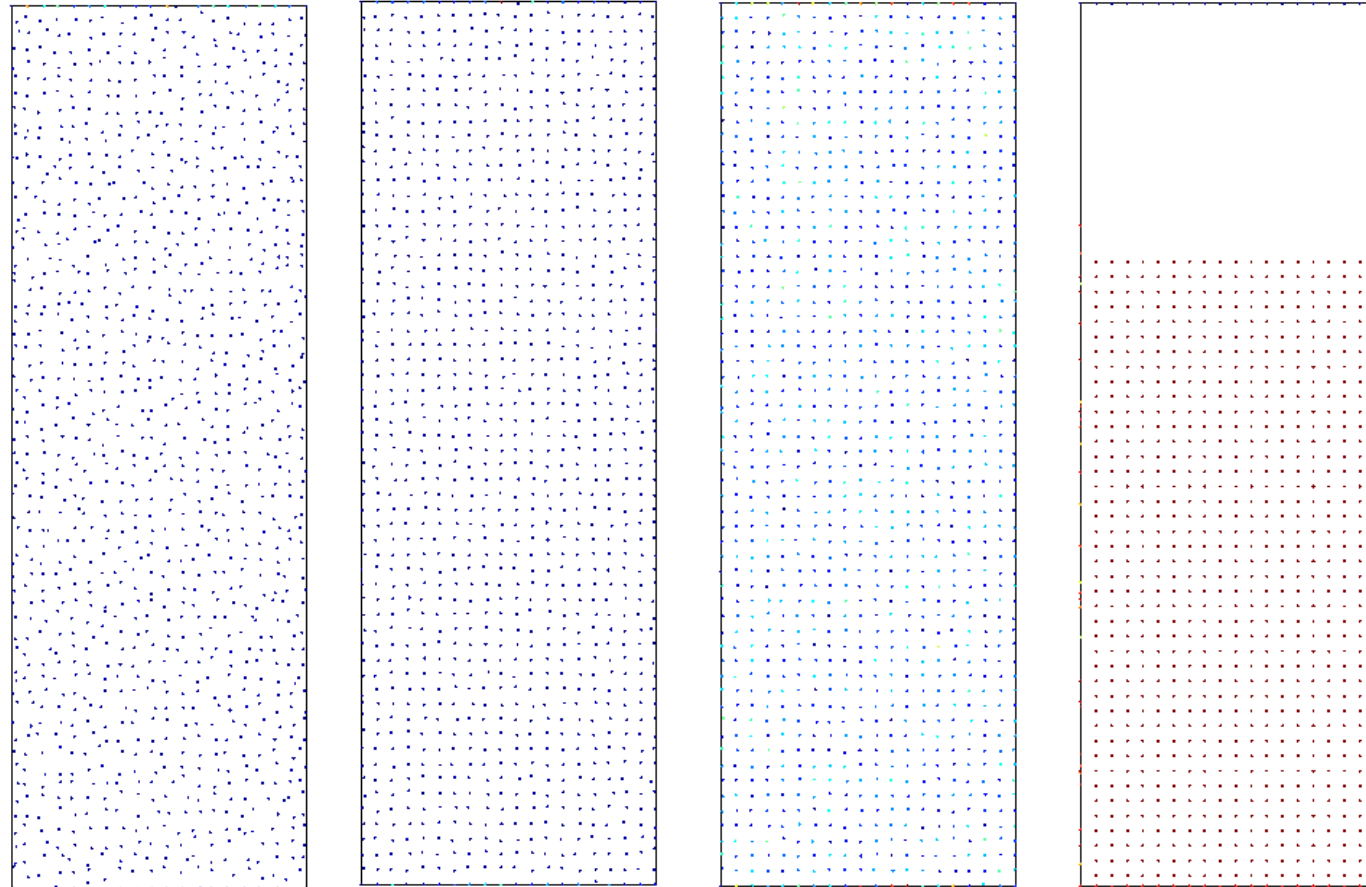


Particle Tracing for Fluid Flow – External forces

The image displays three screenshots of the COMSOL software interface, showing the settings for different external forces applied to particles in a fluid flow model.

- Left Screenshot: Brownian Force**
 - Label: Brownian Force 1
 - Domain Selection: Manual (1)
 - Temperature: Common model input
 - Dynamic viscosity: From material
 - Advanced Settings: Additional input argument to random number generator: $i ds$
 - Particles to affect: All
- Middle Screenshot: Drag Force**
 - Label: Drag Force 1
 - Domain Selection: Manual (1)
 - Coordinate system: Global coordinate system
 - Drag law: Stokes
 - Velocity: User defined (0, 2e-5, 0)
 - Dynamic viscosity: From material
 - Density: From material
- Right Screenshot: Gravity Force**
 - Label: Gravity Force 1
 - Domain Selection: Manual (1)
 - Coordinate system: Global coordinate system
 - Gravity vector: $\mathbf{g} = \begin{matrix} 0 & x \\ -g_const & y \end{matrix} \text{ m/s}^2$
 - Density: From material
 - Affected Particles: All

Particle Tracing for Fluid Flow – External forces



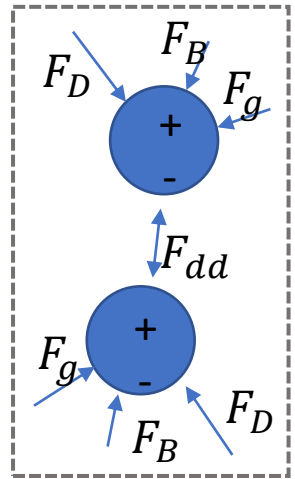
$$r_p = \{100 \text{ nm}, 500 \text{ nm}, 1 \mu\text{m}, 500 \mu\text{m}\}$$

Particle Tracing for Fluid Flow

Inter-particle force

Inter-particle force (F_{dd})

$$F_{dd} = \frac{15 (p_1 \cdot r) (p_2 \cdot r)}{4\pi\epsilon_0 r^7} r - \frac{3 [p_1 (p_2 \cdot r) + p_2 (p_1 \cdot r) + r (p_1 \cdot p_2)]}{4\pi\epsilon_0 r^5}$$



Electrostatic

$$-\nabla \cdot (\epsilon_0 \nabla V - \mathbf{P}) = \rho_c$$

$$P = P_s L (|\mathbf{E}_{eff}|) \frac{\mathbf{E}_{eff}}{|\mathbf{E}_{eff}|}$$

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

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

Particle Tracing for Fluid Flow – Interparticle force

Model Builder

- ParticleTracingmomoria4.mph (root)
 - Global Definitions
 - Parameters 1
 - Default Model Inputs
 - Materials
 - Component 1 (comp1)
 - Definitions
 - Variables 1
 - Boundary System 1 (sys1)
 - View 1
 - Geometry 1
 - Materials
 - Particle Tracing for Fluid Flow (fpt)
 - Wall 1
 - Particle Properties 1
 - Drag Force 1
 - Brownian Force 1
 - Particle Counter 1
 - Accumulator 1
 - Symmetry 1
 - Gravity Force 1
 - Release from Grid 1
 - Particle-Particle Interaction 1
 - Outlet 1
 - Electrostatics (es)
 - Charge Conservation 1
 - Zero Charge 1
 - Initial Values 1
 - Ground 1
 - Terminal 1
 - Charge Conservation, Ferroelectric 1
 - Mesh 1
- Study 2
 - Parametric Sweep
 - Step 1: Time Dependent
 - Solver Configurations
 - Job Configurations
- Results

Settings Properties

Charge Conservation, Ferroelectric

Equation

Ferroelectric Material Properties

$\mathbf{P} - \mathbf{P}_{an}(\mathbf{E}_{eff}) = 0$

Hysteresis Jiles-Atherton model

— An hysteretic polarization

$\mathbf{P}_{an} = P_{sat} L\left(\frac{\mathbf{E}_{eff}}{a}\right) \frac{\mathbf{E}_{eff}}{|\mathbf{E}_{eff}|}$

Saturation polarization:

P_{sat} User defined

Psat C/m²

An hysteretic polarization shape:

Langevin function

$L^{mn} = L\left(\frac{|\mathbf{E}_{eff}|}{a^{mn}}\right) \delta^{mn}, \quad L(x) = \coth(x) - \frac{1}{x}$

Domain wall density:

a From initial susceptibility

$a = \frac{P_{sat}}{3\epsilon_0} \chi_0^{-1}$

Initial electric susceptibility:

χ_0 User defined

chie0 1

Isotropic

— Effective electric field

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

Inter-domain coupling:

α User defined

a m/F

Isotropic

Graphics

Messages Progress Log Table 1

COMSOL Multiphysics 5.6.0.401
 [Jun 18, 2021 9:52 AM] Opened file: C:\Users\curro\Documents\MUCOM\Asignaturas\SegundoSe
 [Jun 18, 2021 10:48 AM] Saved file: C:\Users\curro\Documents\MUCOM\Asignaturas\SegundoSe

Particle Tracing for Fluid Flow – Interparticle force

Settings Properties

Stationary

Compute Update Solution

Label: Stationary

Study Settings

Results While Solving

Physics and Variables Selection

Modify model configuration for study step

Physics interface	Solve for	Discretization
Particle Tracing for Fluid Flow (fpt)	<input type="checkbox"/>	Physics settings
Electrostatics (es)	<input checked="" type="checkbox"/>	Physics settings

Values of Dependent Variables

Mesh Selection

Adaptation and Error Estimates

Study Extensions

Settings Properties

Time Dependent

Compute Update Solution

Label: Time Dependent

Study Settings

Time unit: s

Output times: range(0,0.1e-3,1e-3) s

Tolerance: Physics controlled

Results While Solving

Physics and Variables Selection

Modify model configuration for study step

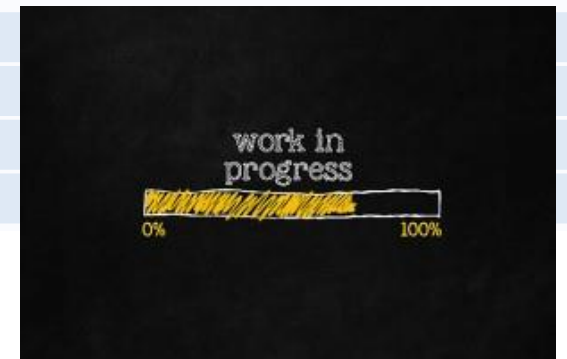
Physics interface	Solve for	Discretization
Particle Tracing for Fluid Flow (fpt)	<input checked="" type="checkbox"/>	Physics settings
Electrostatics (es)	<input checked="" type="checkbox"/>	Physics settings

Values of Dependent Variables

Mesh Selection

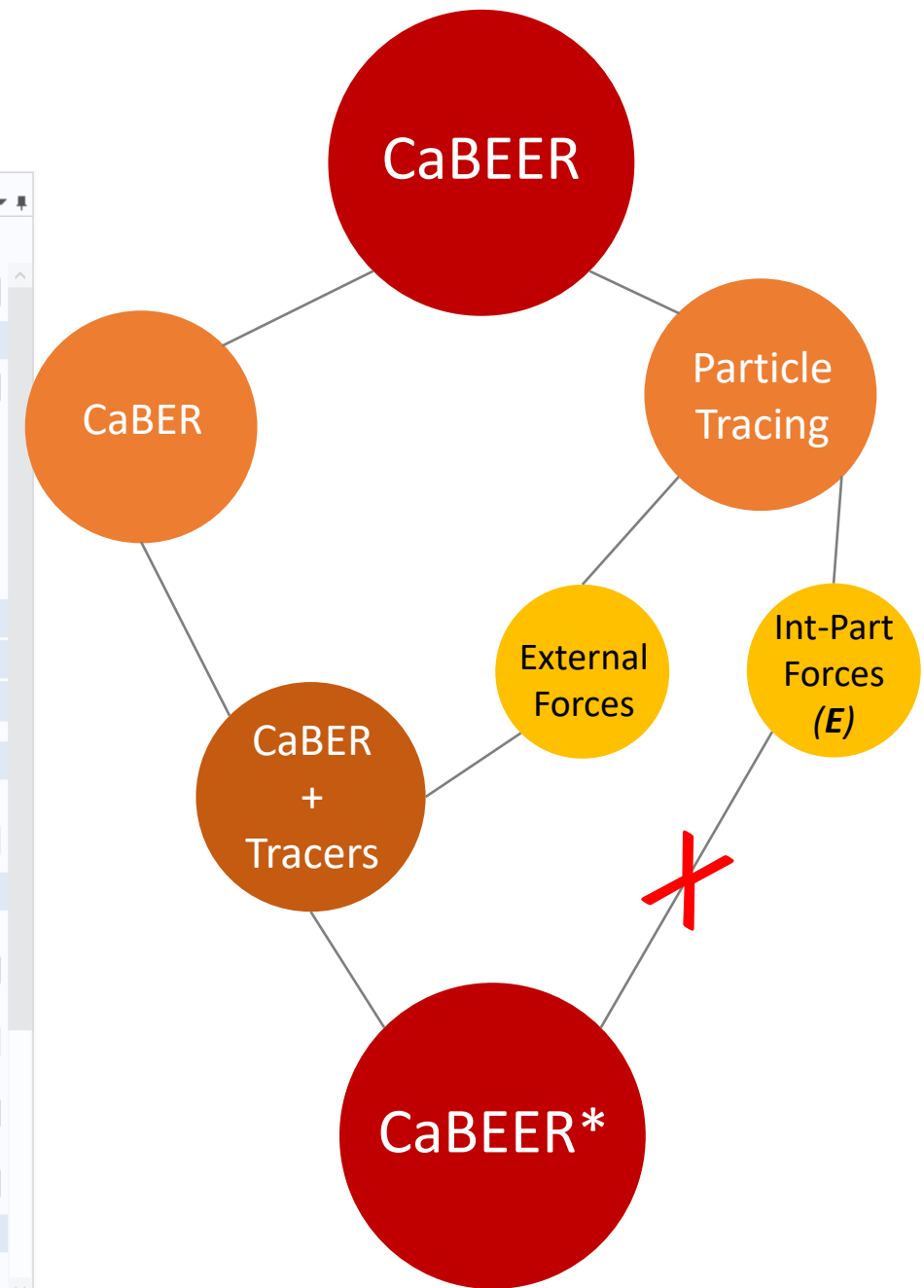
Adaptation

Study Extensions



CaBEER*.mph

The screenshot shows the COMSOL Model Builder interface for a model named 'CaBEER.mph'. The left-hand tree view shows the model structure, with 'Drag Force 1' selected under 'Particle Tracing for Fluid Flow (fpt)'. The right-hand pane displays the 'Settings' for 'Drag Force 1', including domain selection, model input, and drag force parameters like drag law (Stokes), velocity, dynamic viscosity, and density.



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

CaBEER*.mph

Settings
Properties ✕

Time Dependent
= Compute ↻ Update Solution

Label:

▼ Study Settings

Time unit:

Output times: s

Tolerance:

▷ Results While Solving

▼ Physics and Variables Selection

Modify model configuration for study step

▶▶	Physics interface	Solve for	Discretization
	Laminar Flow (spf)	<input type="checkbox"/>	Physics settings ▼
	Phase Field (pf)	<input type="checkbox"/>	Physics settings ▼
	Particle Tracing for Fluid Flow (fpt)	<input checked="" type="checkbox"/>	Physics settings ▼

▶▶	Multiphysics couplings	Solve for
	Two-Phase Flow, Phase Field 1 (tpf1)	<input checked="" type="checkbox"/>

CaBEER-APP

CaBEER_app.mph - TFM MUCOM 20/21 - Francisco J. Galindo-Rosales

File CaBEER Model Documentation

Geometry Simulation

Design Run

2D - Domain design

Length: m

Radius liquid domain: m

Radius air domain: m

Surface Tension

By defect, surface tension is constant:

Surface tension (Cte): N/m

Do you want to consider Marangoni Effects?

Introduce the surface tension expression:

N/m

Viscosity

Liquid viscosity: Pa·s

Density

Liquid density: kg/m³

Parametric Sweep Liquid Properties

Particle Tracing

Electric Field

Surface tension [N/m]: Start: End: Step:

Viscosity [Pa·s]: Start: End: Step:

Information

Last computation time:

galindo@fe.up.pt

sigma2(3)=0.07 Time=4E-5 s

Surface: Volume fraction of fluid 1 (1) Contour: Volume fraction of fluid 1 (1)

This APP has been developed by Francisco José Galindo Rosales as part of the dissertation of Master's Degree in Numerical Simulation in Science and Engineering with COMSOL Multiphysics (MUCOM), 2020/21.

Last update: 20/6/2021

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

Acknowledgements

Author would like to acknowledge the financial support from FCT, COMPETE and European Union (FEDER) through project POCI-01-0145-FEDER-030765 (RheoOptimized2Dinks) and Principal Investigator Grant 2020.03203.CEECIND (EHDViscoElastic).



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

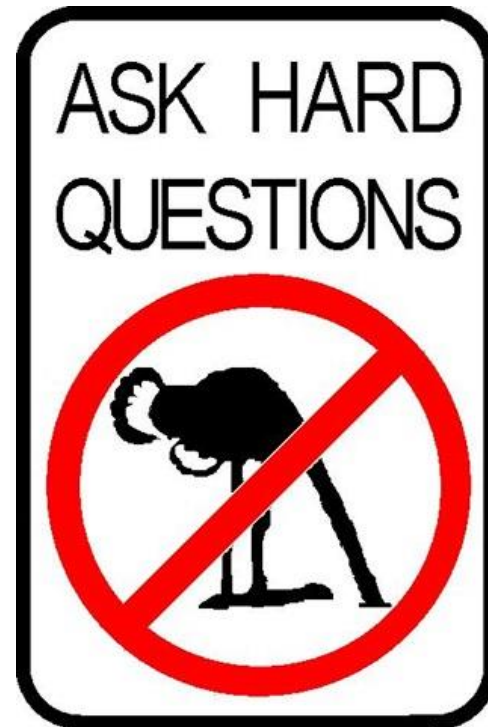
Author: Francisco José Galindo Rosales

Supervisor: Emilio Ruiz Reina

25 de Junio de 2021



UNIVERSIDAD DE MÁLAGA | uma.es



F.J. Galindo-Rosales

Transport Phenomena Research Center
Chemical Engineering Department.
Faculty of Engineering of the University of Porto
R. Dr. Roberto Frias s/n, 4200-465 Porto (Portugal)
galindo@fe.up.pt



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

Francisco José Galindo Rosales

Emilio Ruiz Reina

25 de Junio de 2021



UNIVERSIDAD
DE MÁLAGA



uma.es