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1 **Application of a multiscale approach for modelling the rheology of complex fluids**
2 **in industrial mixing equipment**

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9 Many industrial sectors, like the personal care one, make wide use of mixing processes that
10 involve complex fluids. However, modelling the rheology of these fluids is still challeng-
11 ing due to their non-Newtonian behaviour, which depends also on the local composition.
12 Computational tools such as Dissipative Particle Dynamics (DPD) have been already used
13 to calculate the equilibrium properties of these systems. Moreover, different works have
14 been focused on the calculation of transport properties from these mesoscale DPD simula-
15 tions. Multiscale approaches have been proposed to couple rheological information from
16 DPD with Computational Fluid Dynamics (CFD) simulations. The CFD technique repro-
17 duces the macroscale piece of equipment, implementing a rheology model built using the
18 Gaussian Process Regression (GPR), a mathematical tool related to machine learning. In
19 this work, such framework is tested on an industrial process, to asses its performance on
20 a realistic application. The investigated system is a solution at a high concentration of
21 Sodium Lauryl Ether Sulfate (SLES) in water under laminar fluid dynamics regime. The
22 results show that the mixture correctly exhibits a shear-thinning behaviour and presents
23 viscosity values in good agreement with rheology experiments. While the feasibility of the
24 coupling approach is shown, further studies on DPD are needed to improve the accuracy
25 and the predictability of the methodology.

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26 I. INTRODUCTION

27 The personal care industry makes extensive use of ionic and non-ionic surfactants mixed with
28 water for the production of everyday items, such as shampoos and soaps. Usually, the final prod-
29 ucts for the consumer market have low to moderate concentrations of surfactants ($\sim 12 - 25\%$)^{1,2}.
30 On the other hand, the semi-finished products present considerably higher concentrations of sur-
31 factants. Consequently, during the production step, a great variety of composition conditions are
32 explored. In these blends, the concentration of surfactants plays a crucial role, due to their capabil-
33 ity of undergoing self-assembly at the microscopic scale³. This process leads to the formation of
34 different microstructures depending on composition, ranging from the micellar one to the hexag-
35 onal, cubic, and lamellar ones^{4,5}. For this reason, these fluids are often referred to as structured
36 fluids or complex fluids. The self-assembly occurs also in solutions of water and Sodium Lauryl
37 Ether Sulfate (SLES)³⁻⁵, one of the most commonly used surfactants for personal care products.
38 The presence of microstructures influences greatly the rheology of complex fluids, whose appar-
39 ent viscosity depends on the composition and on the shear rate^{3,4}. As a result, building a model
40 for this rheological behaviour is considerably challenging and requires a significant amount of
41 experimental data.

42 The continuous advances in the field of computational methods can be a great aid to the mod-
43 elling process. Various simulation techniques allow the reproduction of the features of the fluids,
44 from the microstructures at the mesoscale to the macroscopic fluid dynamics in the industrial
45 equipment. In particular, Dissipative Particle Dynamics (DPD) is a computational technique that
46 employs coarse-graining (CG) to describe the molecules in a fluid. The CG description leads to a
47 reduction of the required computational resources when compared to other atomistic techniques,
48 such as Molecular Dynamics (MD). This is due to the reduction of the degrees of freedom, which
49 allows to explore higher spatial and temporal scales while retaining a certain degree of chemical
50 specificity. The DPD technique has already been proven to be able to reproduce a variety of mi-
51 crostructures for complex fluids^{6,7}. The parameterization of a DPD fluid is a vibrant field of study
52 and various approaches were proposed over the years. Since the initial developments of the tech-
53 nique, Groot and Warren⁸ built the parameter set for a simple fluid to match the compressibility
54 of water. Moreover, they proposed a method based on Flory-Huggins theory of polymer solutions
55 to derive the interaction parameters for systems with large molecules⁸. This approach found wide
56 usage in the literature in numerous different applications, like surfactants in oil/water systems⁹,

57 phase diagrams for ternary mixtures⁶ or polymer solutions¹⁰. An automated approach to build the
58 coarse-grained model and identify the parameters was developed by Fraaije *et al.*¹¹ and recently
59 tested on interfacial systems^{12,13}. A parameterization method for small molecules based on fitting
60 the partition coefficients in water-octanol was proposed by Anderson *et al.*¹⁴. The method pro-
61 duces a set of parameters that can be used for different molecules and has been already used to
62 simulate alkyl surfactants. Among these, there was an interest in investigating the phase diagram
63 for solutions of surfactants in water¹⁵, in calculating equilibrium properties^{16,17} and the effect of
64 cosurfactants¹⁸. These studies, though, analyzed low concentrations of alkyl surfactants in water,
65 exploring only the typical final formulations for the consumer market. Moreover, they focused on
66 equilibrium properties, leaving aside the calculation of transport properties, such as diffusion coef-
67 ficients and viscosity. Nonetheless, since its development, DPD has been considered a promising
68 tool for the evaluation of transport properties for colloidal systems^{19,20} and polymer solutions²¹.
69 Various methods have been employed to calculate the viscosity of a DPD fluid²². Simple fluids
70 exhibit Newtonian behaviour, and their viscosity can be evaluated both with equilibrium^{23,24} and
71 non-equilibrium²² techniques. On the other hand, non-equilibrium simulations are necessary to in-
72 vestigate shear-dependent rheology, typical of complex fluids^{7,25–27}. These methods exhibit high
73 uncertainty in viscosity values for low shear rate values^{25,28} and bring to a rise in temperature and
74 viscosity for high shear²², which is unphysical in many cases⁷. To have a better description of
75 transport properties Junghans, Praprotnik, and Kremer²⁹ proposed a modification to the standard
76 DPD thermostat, to include the effect of velocity components other than the radial one. For the
77 same reason, increment of the dissipative coefficient γ was investigated²² and *ad hoc* thermostats
78 have been developed^{30,31}.

79 While atomistic methods are helpful in calculating the properties of fluids, other techniques are
80 instead suited to obtain useful information for design and optimization at the process scale. Among
81 these, Computational Fluid Dynamics (CFD) has been used to simulate a great variety of applica-
82 tions, including mixing ones^{32,33}. Hence, studies were already conducted on static mixers^{34–36}, a
83 piece of equipment often used to produce non-Newtonian solutions of surfactants in water.

84 Using the just described techniques, Zhao *et al.*³⁷ proposed a multiscale approach to simulate
85 the behaviour of non-Newtonian fluids. The method uses DPD simulations to compute the vis-
86 cosity of the fluid at different shear rates, generating a dataset used to build the rheology model.
87 This latter step is performed using the Gaussian Process Regression (GPR), a mathematical and
88 statistical tool that belongs to the family of machine learning techniques. The GPR is then directly

89 coupled with the CFD simulation, with the model that takes the shear rate values from the latter
90 as input and gives the corresponding apparent viscosity in output. This multiscale approach was
91 tested on a polymer melt³⁷ and on a diluted polymer solution³⁸ with promising results, but it was
92 never applied directly to a realistic industrial process.

93 In this work, the rheological behavior of an industrial blend, made of a highly concentrated
94 solution of SLES in water, is reproduced using an automated multiscale approach. The rheological
95 information is extracted by means of a mesoscale DPD simulation and is used to build a rheology
96 model. This is implemented through the GPR in a CFD simulation of the mixing equipment used
97 for the blend production, *i.e.* an SMX static mixer. The DPD model of the fluid is successfully
98 tested by a qualitative reproduction of the SLES/water phase diagram. The CFD is used to evaluate
99 useful fluid dynamics details of the flow inside the static mixer together with the pressure drop
100 across the device. The final values are plausible when compared with results obtained for similar
101 blends in the same piece of equipment.

102 The next three sections are structured as follows: Section II illustrates thoroughly the methods
103 and techniques used in this work, adding also information about the computational details. Sec-
104 tion III reports and comments on the results, focusing on every step of the multiscale approach in
105 different subsections. At last, the conclusions will be presented in Section IV.

106 II. METHODS AND COMPUTATIONAL DETAILS

107 A. The DPD technique

108 The first part of the multiscale approach consists in simulating the fluid at the mesoscale, to ob-
109 tain information about its rheological behaviour. The technique used to perform these mesoscale
110 simulations is the Dissipative Particle Dynamics (DPD), initially developed by Hoogerbrugge
111 and Koelman³⁹ and later improved and formalized in detail by Español, Groot and Warren^{8,40}.
112 The DPD technique employs a coarse-grained description of the molecules, for which atoms are
113 grouped together in particles called beads. These represent the fundamental elements in DPD
114 simulations and can contain a number of atoms, or a number of molecules, depending on the de-
115 sired level of coarse-graining (CG). As a consequence, DPD has the possibility to explore bigger
116 scales in comparison to the full-atom Molecular Dynamics (MD) while keeping low the required
117 computational resources.

118 The dynamics of the DPD particles can be described through Newton's equations of motion:

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i, \quad (1a)$$

119

$$\frac{d\mathbf{v}_i}{dt} = \frac{\mathbf{f}_i}{m_i}, \quad (1b)$$

120 where \mathbf{r}_i is the position of the bead i with mass m_i , and \mathbf{v}_i is its velocity. In the standard DPD
 121 model of a simple fluid, the beads interact with each other through three pairwise forces, that are
 122 summed in the term \mathbf{f}_i of Eq. (1b):

$$\mathbf{f}_i = \sum_{i \neq j} (\mathbf{F}_{ij}^C + \mathbf{F}_{ij}^D + \mathbf{F}_{ij}^R). \quad (2)$$

123 These three forces regulate the interactions of two DPD beads up to a distance equal to the cut-off
 124 radius r_c . More in detail, \mathbf{F}^C is the conservative force:

$$\mathbf{F}_{ij}^C = \begin{cases} a_{ij} \left(1 - \frac{r_{ij}}{r_c}\right) \hat{\mathbf{r}}_{ij} & r_{ij} \leq r_c \\ 0 & r_{ij} > r_c \end{cases}, \quad (3)$$

125 which defines a soft repulsive potential, that allows beads to interpenetrate each other and even
 126 overlap. In this latter case, the conservative force reaches its maximum, which is equal to the
 127 repulsive parameter a_{ij} , whose value depends on the type of beads i and j . The distance between
 128 a pair of particles is identified with $r_{ij} = |\mathbf{r}_{ij}| = |\mathbf{r}_i - \mathbf{r}_j|$ and $\hat{\mathbf{r}}_{ij} = \mathbf{r}_{ij}/r_{ij}$ is the unit vector repre-
 129 senting the direction that connects the centers of the two beads. The dissipative force \mathbf{F}_{ij}^D and the
 130 random force \mathbf{F}_{ij}^R have the following structure:

$$\mathbf{F}_{ij}^D = -\gamma w^D(r_{ij})(\mathbf{r}_{ij} \cdot \mathbf{v}_{ij}) \hat{\mathbf{r}}_{ij}, \quad (4)$$

131

$$\mathbf{F}_{ij}^R = \sigma w^R(r_{ij}) \frac{\xi_{ij}}{\sqrt{\Delta t}} \hat{\mathbf{r}}_{ij}, \quad (5)$$

132 where $w^D(r_{ij})$ and $w^R(r_{ij})$ are the weight functions, $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$ is the relative velocity between
 133 two beads i and j and ξ_{ij} is a Gaussian white-noise variable with zero mean value and unit variance.
 134 These two forces act like a thermostat, in which \mathbf{F}^D is used to model viscous phenomena and \mathbf{F}^R is
 135 used to model the thermal agitation of the molecules. Español and Warren⁴⁰ showed that to respect
 136 the fluctuation-dissipation theorem the dissipative and random forces must be related, through the
 137 values of the parameters γ and σ and through their weight functions:

$$\sigma^2 = 2\gamma k_B T, \quad (6)$$

138

$$w^D(r_{ij}) = [w^R(r_{ij})]^2 = \begin{cases} \left(1 - \frac{r_{ij}}{r_c}\right)^2 & r_{ij} \leq r_c \\ 0 & r_{ij} > r_c \end{cases}. \quad (7)$$

139 These equations ensure the conservation of the energy in the system, in which the two forces act
 140 properly as a thermostat. Moreover, the relation between \mathbf{F}^D and \mathbf{F}^R results in momentum con-
 141 servation and correct hydrodynamic behavior of the DPD fluids for sufficiently large scales^{37,41}.

142 Due to its coarse-grained nature, the DPD model is based on reduced units. It is possible to
 143 retrieve the values in physical units from the DPD reduced units through the use of conversion
 144 factors. The values of these factors depend on the coarse-graining level of the model, but their
 145 identification for a given system is not trivial²⁷. While some procedures were developed for equi-
 146 librium simulations and simple fluids, in the case of non-equilibrium simulations it does not exist
 147 a well-established methodology. The approach chosen for the work here presented is based on
 148 matching the properties of interest for the systems studied. Hence, the conversion factors are
 149 identified in order to match the viscosity of the system at a given shear rate:

$$\mu_{\text{cf}} = \frac{\mu}{\mu_{\text{DPD}}}, \quad (8a)$$

150

$$\dot{\gamma}_{\text{cf}} = \frac{\dot{\gamma}}{\dot{\gamma}_{\text{DPD}}}, \quad (8b)$$

151

$$\mathcal{E}_{\text{cf}} = \frac{\mathcal{E}}{\mathcal{E}_{\text{DPD}}} = \frac{k_B T}{k_{B,\text{DPD}} T_{\text{DPD}}}. \quad (8c)$$

152 In Eq. (8) the subscript ‘‘cf’’ indicates the conversion factor, while the values in DPD units are
 153 marked with the subscript DPD, and the remaining quantities are expressed in physical units.
 154 Defining also the conversion factor for a third quantity, in this case the energy in Eq. (8c), it is
 155 possible to derive the conversion factor for any physical quantity. Considering that the standard
 156 model of the DPD is isothermal, it was possible to establish the energy of the system starting from
 157 a reference temperature.

158 B. Non-equilibrium simulations

159 To simulate a fluid under shear it is possible to apply the Lees-Edwards boundary conditions
 160 (LEBC)⁴², which is used to obtain the velocity profile corresponding to the desired shear rate

161 inside a periodic box. The LEBC method was originally developed and widely used in the context
 162 of MD simulation, but its implementation has been already studied and used in conjunction with
 163 DPD in the past^{7,22,27}. From such kind of simulation it is possible to obtain the pressure tensor \mathbf{P} ,
 164 computed according to the following equation, in which i and j identify different beads:

$$\mathbf{P} = \frac{1}{V} \sum_{i=1}^N m_i \mathbf{v}_i \mathbf{v}_i + \frac{1}{V} \sum_{j>i}^N \sum_{i=1}^{N-1} \mathbf{r}_{ij} \mathbf{F}_{ij}^T. \quad (9)$$

165 The apparent viscosity of the DPD fluid can be calculated from the elements of the pressure tensor:

$$\mu = -\frac{P_{xy}}{\dot{\gamma}}, \quad (10)$$

166 where P_{xy} is the non-diagonal component of the pressure tensor relative to the plane in which the
 167 shear $\dot{\gamma}$ is applied.

168 The DPD simulations were performed using the open-source software LAMMPS⁴³ (Large-
 169 scale Atomic/Molecular Massively Parallel Simulator). For non-equilibrium simulations, Lagrangian-
 170 Rhomboid boundary conditions (LRBC) are implemented in LAMMPS. The LRBC are equivalent
 171 to the LEBC as representation for a simple shear flow^{44,45} and the main difference consists in how
 172 the shear is imposed. For $\dot{\gamma} = \partial v_x / \partial y \neq 0$ using the LEBC, the shear is imposed using a “sliding
 173 brick” approach: the periodic images below and above the simulation box are displaced at $\pm L \dot{\gamma} \Delta t$
 174 in respect to the box itself. The position and velocity of the particles that cross the y boundaries
 175 are set in order to take into account the different values of v_x in the periodic images. Moreover, the
 176 interaction between two particles separated by a boundary is corrected to consider the displace-
 177 ment of the periodic boxes. To obtain the desired velocity profile using the LRBC instead, the
 178 box itself is deformed, as illustrated in Fig. 1, with a rate corresponding to the desired shear. The
 179 deformation induces a perturbation in the velocity of the DPD beads and under the condition of
 180 linear profile for the velocity within the simulation box, the Eq. (10) can be used to calculate the
 181 apparent viscosity.

182 In the approach here described an initial equilibrium simulation is conducted, in order to save
 183 the state of the DPD fluid that reached a dynamic equilibrium condition. This state can be used
 184 as a starting point since it allows to skip the repetition of the equilibration step for every non-
 185 equilibrium simulation. Consequently, the LRBC are directly applied to the equilibrated fluid in
 186 the box, imposing the desired shear rate. Due to the rise in temperature resulting from the imposi-
 187 tion of the shear rate on the box, the SLLOD equations of motion were used, which in LAMMPS

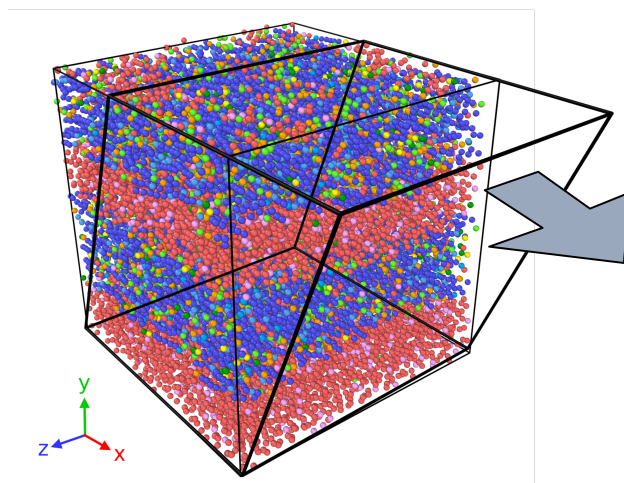


FIG. 1. Illustration of the deformation resulting from the imposition of the LRBC on a DPD box.

188 implement a Nose-Hoover thermostat. This approach is widely used in Molecular Dynamics^{44,45},
 189 and has been lately adopted in some works to perform non-equilibrium DPD simulation with
 190 shear⁴⁶.

191 This paragraph reports the parameters that are common to all the DPD simulations of the
 192 present work. In particular, the value of numerical density for the beads is $\rho_{\text{DPD}} = 3$ and all
 193 the bead types have unitary mass in DPD units. The simulation domain is a cubic box, with a side
 194 of length $L = 40$ (DPD units) used to test the parameters (as described in Section III A) and one of
 195 length $L = 20$ (DPD units) used to carry out the non-equilibrium simulations. The velocity-Verlet
 196 algorithm was used to integrate the equations of motion in all the DPD simulations with a timestep
 197 $\Delta t = 0.01$ (DPD units).

198 C. Miraspec UB75 model

199 The modeled fluid is the Miraspec UB75, a three-component mixture with composition re-
 200 ported in Table I.

201 Besides water, the table reports the use of other two main components:

- 202 • The Inter ESA-70 is a mixture of SLES (Sodium Lauryl Ether Sulfate) at 70% in water,
 203 whose main function is cleansing.
- 204 • CME/A2 is cocamide monoethanolamine (CMEA), used to control foaming, viscosity, and

TABLE I. Composition of the blend Miraspec UB75 used for the DPD simulations.

Component	Mass fraction
Inter ESA-70	0.72
CME/A2	0.08
Water	0.20

205 mildness of the product.

206 As depicted in Fig. 2 and Fig. 3, both SLES and CMEA have an alkyl tail, which can be formed
 207 by a different number of carbon atoms. In particular in Table II and Table III are reported the per-
 208 centages of the molecules for every length of the alkyl chain. These characterize the components
 209 of the blend and they are used to calculate the numerical concentrations of the beads in the DPD
 210 simulations of the Miraspec UB75.

TABLE II. Percentage of SLES molecules with a specific length of the alkyl chain, expressed in number of carbon atoms, in the Inter ESA-70 component.

Number of Carbon atoms	Percentage in Inter ESA-70
12	70%
14	30%

TABLE III. Percentage of CMEA molecules with a specific length of the alkyl chain, expressed in number of carbon atoms, in the CME/A2 component.

Number of Carbon atoms	Percentage in CME/A2
8	6%
10	6%
12	50%
14	18%
16	9%
18	11%

211 Again in Fig. 2, it is shown that the SLES molecule can have a different number of ethoxyl (EO)

212 groups $(\text{CH}_2\text{CH}_2\text{O})_n$. While the Miraspec UB75 contains only molecules of SLES with a single
 213 EO group, the phase diagram reported in the work of Li *et al.*³ refers to SLES molecules with
 214 three EO groups. Consequently, the molecule used for the validation in Section III A contained
 215 two more $[\text{CH}_2\text{OCH}_2]$ beads than the one depicted in Fig. 2.

216 The process of developing the final model went through different steps. Initially, a DPD model
 217 for SLES and water is tested, using the set of parameters to reproduce the phase diagram of the
 218 mixture. Then a coarse-grained model for CMEA is developed with the same parametrization
 219 method, and the correct reproduction of the microstructure of the blend is used as a test. In the
 220 end, the non-equilibrium simulations are performed with the developed DPD model, to obtain the
 221 information on the rheology of the fluid. It must be remarked that it does not exist a unique stan-
 222 dardized process to develop the parameters of a DPD model. Hence, depending on the system
 223 features and the level of coarse-graining, different methods can be used. Anderson *et al.*¹⁴ devel-
 224 oped a parametrization scheme based on the water-octanol partition coefficients. The parameters
 225 obtained with this technique have been used to simulate micellar blends of alkyl sulfate, alkyl
 226 ethoxylate and alkyl ethoxy sulfate surfactants^{14–18}. In this work we used the latter approach to
 227 model the SLES molecules, adopting the same CG level depicted in Fig. 2.

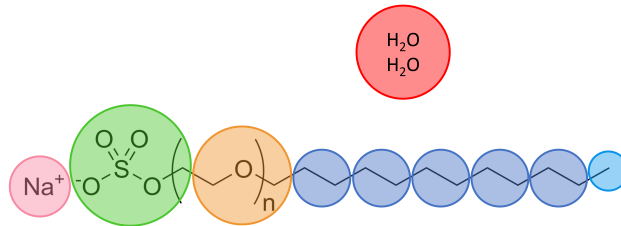


FIG. 2. Coarse graining model adopted for water and SLES molecules¹⁵. Changing the length of the alkyl tail results in the addition or the subtraction of $[\text{CH}_2\text{CH}_2]$ beads.

228 The full list of conservative parameters a_{ij} and cutoff radii $r_{c,ij}$, reported in Table IV, was
 229 obtained from previous works^{14,15}, while in Table V are reported the dissipative parameters γ and
 230 the stochastic one σ , common to all the beads.

TABLE IV: List of conservative repulsive parameter a_{ij} and cutoff radius $r_{c,ij}$ for each pair of beads.

Bead i	Bead j	conservative coefficient a_{ij}	cutoff radius $r_{c,ij}$
[H ₂ O]	[H ₂ O]	25.0	1.000
[CH ₃]	[CH ₃]	24.0	0.955
[CH ₂ CH ₂]	[CH ₂ CH ₂]	22.0	1.074
[CH ₂ OCH ₂]	[CH ₂ OCH ₂]	25.5	1.116
[CH ₂ OSO ₃ ⁻]	[CH ₂ OSO ₃ ⁻]	13.30	1.234
[Na]	[Na]	25.00	1.000
[CH ₃ CH ₂]	[CH ₃ CH ₂]	22.00	1.098
[CH ₂ CONHCH ₂]	[CH ₂ CONHCH ₂]	22.00	1.218
[CH ₂ OH]	[CH ₂ OH]	14.00	0.980
[H ₂ O]	[CH ₃]	45.00	0.977
[H ₂ O]	[CH ₂ CH ₂]	45.00	1.037
[H ₂ O]	[CH ₃]	24.00	1.058
[H ₂ O]	[CH ₂ OCH ₂]	17.90	1.117
[H ₂ O]	[CH ₂ OSO ₃ ⁻]	25.00	1.000
[H ₂ O]	[Na]	45.00	1.049
[H ₂ O]	[CH ₃ CH ₂]	19.00	1.109
[H ₂ O]	[CH ₂ OH]	14.50	0.990
[CH ₃]	[CH ₂ CH ₂]	23.00	1.014
[CH ₃]	[CH ₂ OCH ₂]	28.50	1.020
[CH ₃]	[CH ₂ OSO ₃ ⁻]	28.50	1.071
[CH ₃]	[Na]	45.00	0.962
[CH ₃]	[CH ₃ CH ₂]	23.00	1.026
[CH ₃]	[CH ₂ CONHCH ₂]	32.00	1.086
[CH ₃]	[CH ₂ OH]	26.00	0.967
[CH ₂ CH ₂]	[CH ₂ OCH ₂]	28.50	1.095
[CH ₂ CH ₂]	[CH ₂ OSO ₃ ⁻]	28.50	1.154
[CH ₂ CH ₂]	[Na]	45.50	1.037

Table IV (continued): List of conservative repulsive parameter a_{ij} and cutoff radius $r_{c,ij}$ for each pair of beads.

Bead i	Bead j	conservative coefficient a_{ij}	cut-off radius $r_{c,ij}$
[CH ₂ CH ₂]	[CH ₃ CH ₂]	22.00	1.086
[CH ₂ CH ₂]	[CH ₂ CONHCH ₂]	32.00	1.146
[CH ₂ CH ₂]	[CH ₂ OH]	26.00	1.027
[CH ₂ OCH ₂]	[CH ₂ OSO ₃ ⁻]	15.50	1.175
[CH ₂ OCH ₂]	[Na]	24.00	1.058
[CH ₂ OCH ₂]	[CH ₃ CH ₂]	28.50	1.107
[CH ₂ OCH ₂]	[CH ₂ CONHCH ₂]	15.73	1.167
[CH ₂ OCH ₂]	[CH ₂ OH]	25.00	1.059
[CH ₂ OSO ₃ ⁻]	[Na]	17.90	1.117
[CH ₂ OSO ₃ ⁻]	[CH ₃ CH ₂]	28.50	1.166
[CH ₂ OSO ₃ ⁻]	[CH ₂ CONHCH ₂]	13.57	1.226
[CH ₂ OSO ₃ ⁻]	[CH ₂ OH]	21.70	1.048
[Na]	[CH ₃ CH ₂]	45.00	1.049
[Na]	[CH ₂ CONHCH ₂]	18.33	1.109
[Na]	[CH ₂ OH]	25.80	0.990
[CH ₃ CH ₂]	[CH ₂ CONHCH ₂]	32.00	1.158
[CH ₃ CH ₂]	[CH ₂ OH]	26.00	1.038
[CH ₂ CONHCH ₂]	[CH ₂ OH]	26.00	1.099

TABLE V. DPD parameter in common to every bead of the Miraspec UB75 blend.

Parameter	Value (DPD units)
γ	10.125
σ	4.5

231 The bonded interactions between two consecutive beads are modeled using the harmonic po-
 232 tential in Eq. (11),

$$E_{\text{bond}} = \frac{1}{2}k_{\text{bond}}(r - r_0)^2, \quad (11)$$

233 with $k_{\text{bond}} = 150$ (DPD units) for all the bonds and an equilibrium distance calculated according
 234 to the following equation¹⁶:

$$r_0 = 0.1(n_i + n_j) - 0.01 , \quad (12)$$

235 where n_i and n_j are the number of heavy atoms linearly bonded in the i and j bead respectively.
 236 According to this rule, $n_i = 4$ for the sulfate bead, with two oxygen atoms that are considered
 237 “branched” from the linear chain. The model also includes an angle harmonic potential, that
 238 involves three beads interacting according to the formula:

$$E_{\text{angle}} = \frac{1}{2}k_{\text{angle}}(\theta - \theta_0)^2 , \quad (13)$$

239 where θ is the angle between two adjacent bonds, $k_{\text{angle}} = 5$ (DPD units) and $\theta_0 = 180^\circ$ for all the
 240 the interactions.

241 Within the model, it is particularly interesting the treatment of the charged beads, *i.e.* sodium
 242 ion and sulfate group. The standard DPD model allows overlapping of the beads, but in the case of
 243 $r_{ij} = 0$ the Coulombic potential diverges, leading to the creation of artificial ionic pairs^{47,48}. Previ-
 244 ous works on analogous systems adopted a smeared charge approach to overcome this issue^{15–18}.
 245 The same approach was kept in this work, using a Slater-type charge smearing formulated by
 246 González-Melchor *et al.*⁴⁸:

$$E_{\text{el}} = \frac{Cq_iq_j}{\epsilon_r} \left(1 - \left(1 + \frac{r_{ij}}{\lambda} \exp(-2r_{ij}/\lambda) \right) \right) \quad r_{ij} \leq r_{c,\text{el}} , \quad (14)$$

247 where, following the implementation of Anderson *et al.*¹⁶, the decay length is $\lambda =$
 248 $1/0.929$ (DPD units) and $r_{c,\text{el}} = 3$ (DPD units). The latter parameter, $r_{c,\text{el}}$, acts like a cutoff for
 249 the treatment of the electrostatic forces. When $r_{ij} \leq r_{c,\text{el}}$ the interaction between two beads is eval-
 250 uated through Eq. (14), while for $r_{ij} > r_{c,\text{el}}$ the PPPM (particle-particle particle-mesh) solver, in its
 251 LAMMPS implementation, is used to evaluate the electric field. The previous literature focused
 252 on the study of solutions of SLES in water in micellar phases, a microstructure formed for low
 253 concentrations of the surfactant. Consequently, in these previous studies, the value of the dielec-
 254 tric permittivity constant was set equal to the one of water, $\epsilon_r = 78.3$. In the case of the Miraspec
 255 UB75, the concentration of the SLES is substantially higher, hence the value $\epsilon_r = 25$ was used.
 256 This latter value was chosen because it allowed to reproduce qualitatively the microstructures for
 257 different compositions of the mixture of water and SLES, as reported in Section III A.

258 To simulate the CMEA molecules, a new CG representation was developed, as illustrated in
259 Fig. 3.

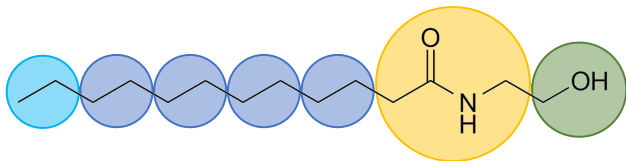


FIG. 3. Coarse graining model developed for CMEA molecules. Changing the length of the alkyl tail results in the addition or the subtraction of $[\text{CH}_2\text{CH}_2]$ beads.

260 The DPD interaction parameters for the beads constituting the CMEA are only in part already
261 present in the literature, in the work of Wand *et al.*¹⁸; the rest were obtained using the same
262 approach, the water/octanol partition method¹⁴, and they were kindly provided by Dr. Richard
263 Anderson. These parameters are relative to the interactions of the $[\text{CH}_2\text{OH}]$ bead present in the
264 CMEA molecule and are also listed in Table IV.

265 The set of conversion factors in Table VI was used for the UB75 blend and it comes from
266 matching one experimental value of viscosity. This approach was chosen due to the current im-
267 possibility of matching all the properties of a fluid with a single set of conversion factors in DPD.
268 This becomes particularly true for transport properties and when performing non-equilibrium sim-
269 ulations. In this case, a linear velocity profile must be obtained in a small box, so the stream
270 velocity must overcome the thermal velocity of the beads. Together with the nature of the DPD
271 forces, this leads to very high shear rates at the macroscale and may result in a shift of the rheol-
272 ogy model. Hence, the identification of conversion factors focused on matching the properties of
273 interest, *i.e.* viscosity and shear rate, also intending to compensate for the described shift to higher
274 shear rates. From the available experiments, the viscosity at the lowest shear rate was matched
275 with the lowest meaningful value of the DPD shear rate. This corresponds to the lowest $\dot{\gamma}_{\text{DPD}}$ that
276 still results in a linear velocity profile from the imposition of the LRBC. For what concerns the en-
278 ergy conversion factor, it was obtained considering the temperature $T = 298.15$ K, the Boltzmann
279 constant $k_B = 1.38 \times 10^{-23} \text{ J} \cdot \text{K}^{-1}$, $T_{\text{DPD}} = 1$, $k_B = 1$ with the application of Eq. (8).

280 The equilibration stage lasted 1.2×10^6 timesteps, while the deformation of the non-equilibrium

TABLE VI. Set of conversion factors used for the Miraspec UB75 DPD model.

μ_{cf} (Pa · s)	$\dot{\gamma}_{\text{cf}}$ (s ⁻¹)	\mathcal{E}_{cf} (J)
2.59	10	4.11×10^{-21}

281 stage was set to 10^6 timesteps. The cumulative average of the DPD viscosity is computed, and its
 282 value at the end of the simulation is extracted.

283 D. Gaussian Process Regression

284 Although the information derived from Dissipative Particle Dynamic simulations is needed to
 285 reproduce the behavior of the fluid at the macroscale, a tight coupling between DPD and CFD is
 286 unfeasible. In such a coupling, the main hindrance would be the computational effort required to
 287 run microscale simulations. For this reason, the development of a kriging strategy to provide an
 288 unbiased rheological relationship is devised. A similar approach was proposed by Zhao *et al.*³⁷,
 289 who used Gaussian Process Regression (GPR)⁴⁹ to link the viscosity values extracted from DPD
 290 with the imposed local shear rate. GPR is a mathematical and statistical tool akin to machine
 291 learning and to grasp the concept behind it, it is possible to think of a distribution over functions.
 292 When there are no training data points, the *prior distribution* is usually a distribution of functions
 293 whose mean is equal to zero and whose standard deviation is unitary. Indeed, for every value of the
 294 independent variable x , the value of y is normally distributed around a mean, with an associated
 295 standard deviation. Hence, it is important to stress that the GPR does not output a functional form
 296 of the target function, and it is instead a statistical model that outputs the predicted y values for
 297 any tested x in input. The shape of the functions sampled from this distribution derives from the
 298 Kernel, which defines the properties, such as derivability, of the mentioned functions. In this work
 299 a Radial Basis Function (RBF), or *squared exponential*, Kernel was used:

$$K(x_i, x_j) = \sigma_f^2 \exp\left(-\frac{d(x_i, x_j)^2}{2l^2}\right), \quad (15)$$

300 where σ_f is the *signal variance*, a pre-factor related to how much the functions vary vertically,
 301 $d(\cdot, \cdot)$ is the Euclidian distance between the two points x_i and x_j , and l is the *characteristic length-*
 302 *scale*⁴⁹. The latter parameter expresses how the functions can vary: a high value of l will output
 303 smoother functions, that do not show rapid variations. Often σ_f and l are referred to as *hyper-*

304 *parameters* since they are free parameters, whose value can be varied and it is usually optimized
 305 through different techniques.

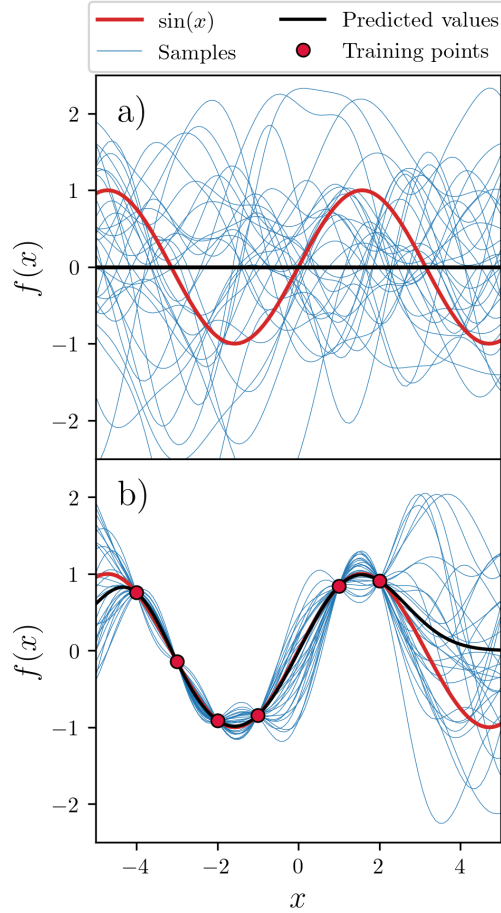


FIG. 4. Result of the GPR on an example function $y = \sin(x)$ with RBF kernel. Different steps are illustrated: a) prior distribution, b) posterior distribution obtained with six training data points. The functions in blue are samples from the distributions of functions.

306 The addition of training points $(x_{\text{train}}, y_{\text{train}})$ to the training data set changes the distribution of
 307 functions, which results in the *posterior distribution*. The effect of adding training data points can
 308 be noticed by comparing Fig. 4.a and Fig. 4.b, whose plots illustrate the use of the GPR on a test
 309 function $y = \sin(x)$. Considering the distribution of functions of a GPR model, it is possible to
 310 take samples from this distribution, analogously to what can be done by sampling a distribution of
 311 numbers. However, in this case, the samples correspond to functions that respect the constraints
 312 imposed by the used kernel and the training data set. Starting from the prior distribution in Fig. 4.a,

313 in which sample functions from the distribution are plotted in blue, the addition of training points
314 forces said functions to pass through them, as in Fig. 4.b. The prediction values, plotted in black,
315 are the result of the regression and they are generated by calculating the mean of the normally
316 distributed functions.

317 Due to the width of the shear rate intervals, the GPR for the simulated systems was performed
318 on the log-space, *i.e.* using the values of $\log(\dot{\gamma})$ vs $\log(\mu)$, with an approach comparable to the
319 one of Zhao *et al.*³⁷.

320 In this work, the Python module *scikit-learn*⁵⁰ was used to perform the GPR step, and in par-
321 ticular to optimize the values of the hyperparameters σ_f and l . After the evaluation of the quality
322 of the regression, the training data set and the values of the hyperparameter are passed to a GPR
323 viscosity model implemented in the CFD code OpenFOAM. This viscosity model works as a func-
324 tion: after reading the GPR hyperparameters, it requires the local value of the strain rate, which
325 is evaluated through the solution of the momentum balance equation, and it provides the viscosity
326 value as output for each cell of the computational domain. The implementation of the GPR in
327 OpenFOAM is written in C++ and it is inspired by freely available implementations on Github⁵¹.

328 E. The CFD model

329 The last step of the multiscale approach is the Computational Fluid Dynamics (CFD) simula-
330 tion, which makes use of the GPR viscosity model derived from the DPD non-equilibrium sim-
331 ulations. As previously mentioned, the CFD simulation can provide information about the fluid
332 dynamics of mixing devices^{36,52}. In this work, this simulation is carried out in isothermal condi-
333 tions, under laminar regimen, and the fluid is considered incompressible. In this attempt to apply
334 the multiscale approach to a complex fluid to test the feasibility, the concentration of the species
335 in the system was considered uniform. As a consequence, the viscosity of the fluid depends only
336 on the strain rate $\dot{\gamma}$, and the system is investigated at the steady state.

337 The CFD simulations were carried out using the software OpenFOAM (version 8)⁵³ and in
338 particular the steady-state solver `simpleFoam`. The pressure-velocity coupling algorithm adopted
339 is the SIMPLEC (consistent SIMPLE).

340 F. Multiscale coupling

341 A linking step between the techniques described in the previous sections was developed, to
 342 build a functional and automated multiscale approach. The coupling is based on an iterative flow
 343 scheme, implemented in Python, reported in Fig. 5, with an approach similar to the one described
 344 in Zhao *et al.*³⁷.

345 The starting point, as in Fig. 5, is a CFD simulation that implements a Newtonian model. The
 346 viscosity value for this Newtonian model can be obtained from an initial DPD simulation, per-
 347 formed with a low value of the shear rate $\dot{\gamma}_{\text{DPD}}$. With the completion of this first CFD simulation,
 348 the loop indicated with the blue arrows in Fig. 5 is initiated. This will be called *outer loop*, and
 349 it starts with the extraction of the interval of the strain rate values from the CFD simulation. The
 350 strain rate interval is then passed to the GPR, which builds the model from the training data set,
 351 *i.e.* the couples of points $(\dot{\gamma}, \mu(\dot{\gamma}))$ obtained from the DPD simulations. Once the model is built,
 352 it takes the strain rate values in input and outputs the corresponding viscosity values (predictions)
 353 together with an associated standard deviation σ . This latter variable is then used to test the quality
 354 of the model in the whole interval. If the σ associated with any viscosity prediction is higher than
 355 a user-set limit σ_{lim} , the quality of the model is deemed not sufficient. In this case, the *inner loop*,
 356 indicated with the orange arrows in Fig. 5, starts and a new DPD simulation is issued. The value of
 357 $\dot{\gamma}_{\text{DPD}}$ to impose for this simulation is the one corresponding to the maximum value of σ obtained
 358 in the tested interval. This iterative process is repeated until the regression is satisfactory, and a
 359 new training data point is added for every cycle of the loop. This makes the algorithm automated,
 360 since a certain number of DPD simulations are launched until the desired accuracy on the shape
 361 of the constitutive relationship is met. When the exit condition for the *inner loop* is respected, the
 362 GPR is implemented in OpenFOAM as a viscosity model, and a new CFD simulation is launched.
 363 The updated strain rate interval, extracted from the last simulation, is compared with the one pre-
 364 viously fed to the GPR. If the new interval is wider than a tolerance set by the user, the GPR model
 365 is tested on the updated interval and the *inner loop* may start again, depending on the values of σ .
 366 The difference between the extremes of the shear rate intervals is calculated as a relative difference
 367 according to the following equations:

$$\epsilon_{\text{min,rel}} = \frac{\dot{\gamma}_{\text{min}}^{(n-1)} - \dot{\gamma}_{\text{min}}^{(n)}}{\dot{\gamma}_{\text{min}}^{(n-1)}}, \quad (16a)$$

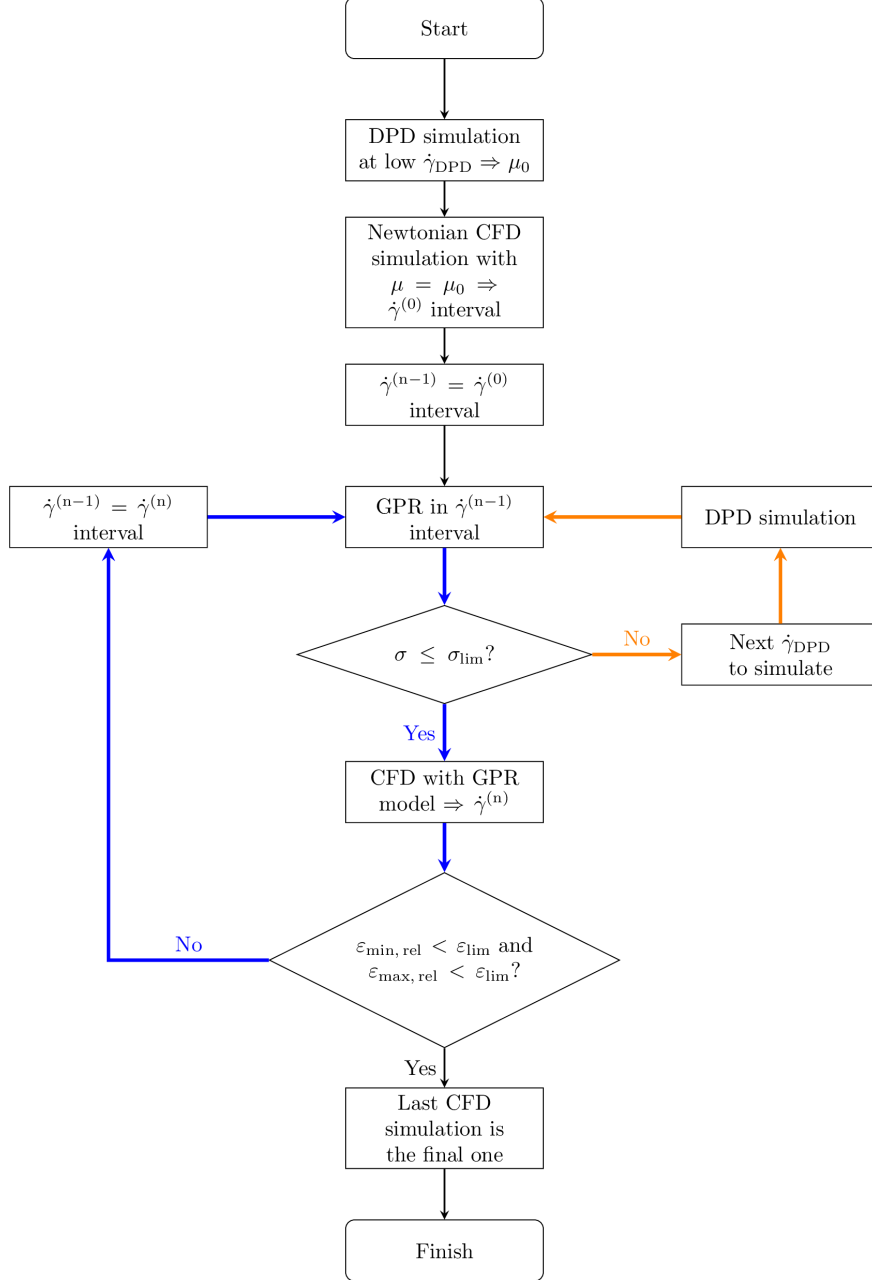


FIG. 5. Flowscheme used in the multiscale coupled approach. The following symbols are used: $\dot{\gamma}_{\text{DPD}}$ is the shear rate used for a DPD simulation, μ_0 is the viscosity obtained from the first DPD simulation, and used to perform the Newtonian CFD simulation, $\dot{\gamma}^{(i)}$ identifies the i -th rate interval from CFD simulations, σ is the standard deviation associated with the regression, σ_{lim} is the user-set limit for said standard deviation, ϵ_{rel} is the relative difference between the extremes of two shear rate intervals as in Eq. (16), and ϵ_{lim} is the user-set limit for said relative differences.

$$\varepsilon_{\max, \text{rel}} = \frac{\dot{\gamma}_{\max}^{(n)} - \dot{\gamma}_{\max}^{(n-1)}}{\dot{\gamma}_{\max}^{(n-1)}}, \quad (16b)$$

369 where $\varepsilon_{\max, \text{rel}}$ and $\varepsilon_{\min, \text{rel}}$ must be smaller than a set limit value ε_{lim} to exit the loop. It must be
 370 stressed that the absolute value is not used in Eq. (16) because the convergence criterion should
 371 discriminate between a wider and a narrower interval. The use of the absolute value will not lead
 372 to convergence in case of a much narrower $\dot{\gamma}^{(n)}$ interval, since it would not take into account the
 373 sign of $\varepsilon_{\max, \text{rel}}$ and $\varepsilon_{\min, \text{rel}}$. For this reason, the order of the terms at the numerator of Eq. (16) is
 374 of paramount importance. Conversely, if the interval is not significantly wider or the quality of the
 375 regression is sufficient, the process exits from the *outer loop*. At this point, the CFD simulation
 376 that was performed last is considered to be the one that reproduces the studied system.

377 G. Sulzer SMX static mixer model

378 The application example selected in this work to test the multiscale coupling procedure is one
 379 step of the production process of the Miraspec UB75, namely the post-mixing section of a blend
 380 reported in Table I. This phase is carried in a static mixer, like the Sulzer SMX, that consists of a
 381 tube filled with mixing elements. Depending on the kind of application, these internal elements
 382 can have different shapes. In the studied equipment there are six identical mixing elements, each
 383 one rotated by 90° axis with respect to the previous, having the z axis as the axis of rotation. Every
 384 element is constituted by inclined bars, as it is possible to notice from Fig. 6. The inclination
 385 of each bar, with respect to both the main flux direction and the adjacent bars, is responsible
 386 for the mixing itself. The main flow gets broken down following smaller flow paths which are
 387 subsequently recombined due to the peculiar geometry of the mixer internals. Still in Fig. 6 is also
 388 displayed an initial empty region of the tube, used to obtain a developed flow at the beginning of
 389 the mixing section. The details of the static mixer geometry are reported in Table VII.

390 The boundary conditions applied to the system are summarised in Table VIII, where the pres-
 391 sure outlet value was kept at zero. The mesh is completely tetrahedral and contains 5118292 cells,
 392 and it has been selected after a grid convergence study. Based on the typical densities of these
 393 blends, $\rho = 1160 \text{ kg m}^{-3}$ was imposed for the CFD simulations.

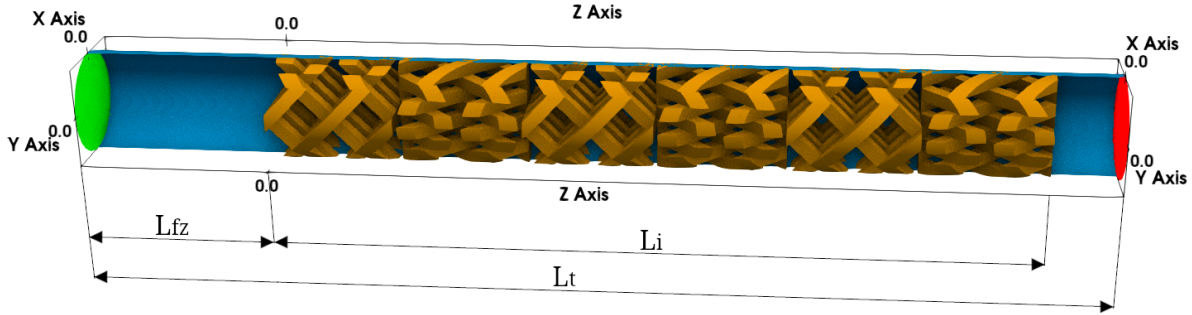


FIG. 6. Geometry of the SMX Sulzer static mixer used in the simulations. The color scheme identifies different regions of the geometry: green for the inlet, red for the outlet, blue for the wall of the tube, and orange for the mixing elements. This color coding is adopted for clarity, but in the actual computational domain used for the simulations the tube (blue) and the internals (orange) are part of the same wall patch, as in Table VIII.

TABLE VII. Geometrical details of the computational domain.

		Symbol	Value
Diameter	(mm)	D	16
Tube length	(mm)	L_t	160
Internals length	(mm)	L_i	122
Number of elements		N_e	6
Number of bars per element		N_b	4
Initial free zone length	(mm)	L_{fz}	30

394 III. RESULTS AND DISCUSSION

395 A. Solvay's UB75 blend: testing the DPD model

396 Before showing the results obtained by the multiscale approach, it is worth to discuss specif-
 397 ically the DPD model and in particular the CG approach reliability. As previously mentioned,
 398 among many available approaches to build a DPD model for a large molecule, in this work we
 399 used the approach of Anderson *et al.*¹⁴ to build the DPD model of the molecules in the Miraspec
 400 UB75 blend^{14,16}. The starting point is the Inter ESA-70, a mixture of Sodium Lauryl Ether Sulfate
 401 (SLES) molecules with different lengths of the alkyl tail. The coarse-grained model of a SLES

TABLE VIII. Boundary conditions used for the CFD simulations with the SMX Sulzer.

	Wall	Inlet	Outlet
		Fixed value	
Velocity	No slip	$U_x, U_y = 0$ $U_z = 1.38 \times 10^{-2} \text{ m s}^{-1}$	Zero gradient
Pressure	Zero gradient	Zero gradient	Fixed value $p = 0 \text{ Pa}$

402 molecule and the DPD parameters reported in Ref. 15 were tested. The DPD model assessment
 403 is carried out through a qualitative comparison between simulation results and the experimental
 404 phase diagram of a SLES/water mixture³. It is important to notice that the mixture reproduced
 405 to test the parameters does not exactly represent the Inter ESA-70. More precisely, the SLES
 406 molecules simulated in this step present a higher number of ethoxyl groups and a different length
 407 of the alkyl chain³. Nonetheless, the ability to reproduce a water/SLES phase diagram can provide
 408 a measure of the quality of the DPD model for these kinds of molecules. The lower side of the
 409 ternary phase diagram in Ref. 3 represents a binary mixture of SLES and water, from which three
 410 regions are identified to conduct the assessment. While for low SLES concentrations (0.00236 –
 411 28% w/w) a micellar phase is found, intermediate SLES concentrations (31.5 – 56% w/w) lead
 412 to the formation of the hexagonal phase and for high SLES concentrations (63 – 70% w/w) a
 413 transition to lamellar phase occurs⁴.

414 One equilibrium DPD simulation in each of these regions is performed, and the resulting mi-
 415 crostructure is qualitatively analyzed. The three DPD simulations performed are summed up in
 416 Table IX, and they resulted in agreement with the phase diagram, as it is possible to see in Fig. 7.

TABLE IX. Values of SLES mass fraction used in the DPD simulation and corresponding expected microstructure according to Refs. 3 and 4.

Expected structure	Simulated SLES mass fraction
Micellar	0.03
Hexagonal	0.45
Lamellar	0.67

417 In particular, to obtain a qualitative confirmation of the hexagonal structure, it was necessary
 418 to conduct a non-equilibrium simulation with an imposed shear rate $\dot{\gamma} = 0.1$ (DPD units) on the
 419 velocity component v_x along the y axis. This kind of behavior was already reported in the literature
 420 for a DPD model that simulates a mixture of water and a tri-block co-polymer⁷. When there is
 421 no shear applied the fluids form a network of worm-like micelles, as in Fig. 7.c. From Fig. 7.d
 422 it is clear how the application of a shear brings to the formation of rodlike micelles, typical of
 423 hexagonal structures.

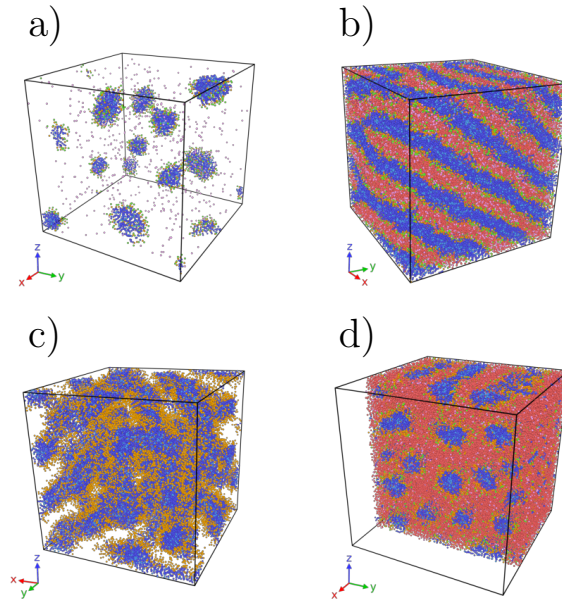


FIG. 7. Resulting microstructures of the DPD simulation performed. SLES mass fraction equal to a) 0.03,
 b) 0.67, c) and d) 0.45. In c) there is no shear applied, the water and the sulfate groups beads are not
 shown to highlight the network formed by the wormlike micelles, while in d) the system is shown after the
 application of a shear of $\dot{\gamma} = 0.1$ (DPD units) along the y axis to the velocity component v_x . To allow the
 micelles visualization, the water beads are not shown in a). To facilitate the visualization of the rodlike
 micelles in d) the box is sliced at 3/4 of its length in the x direction. The color coding of the beads is shown
 in Fig. 2.

424 Having assessed the qualitative capability of the model to predict the microstructure self-
 425 assembly for the binary system made of SLES and water, the addition of the third component
 426 was tested. The CME/A2 component is Cocamide Monoethanolamine (CMEA), whose coarse-
 427 grained model was developed and as described in Section II C with parameters for the DPD forces
 428 retrieved from the literature^{14–16}. In Fig. 8 it is shown that, for the composition in Table I, it is

429 obtained a lamellar microstructure, which is indeed expected for the Miraspec UB75.

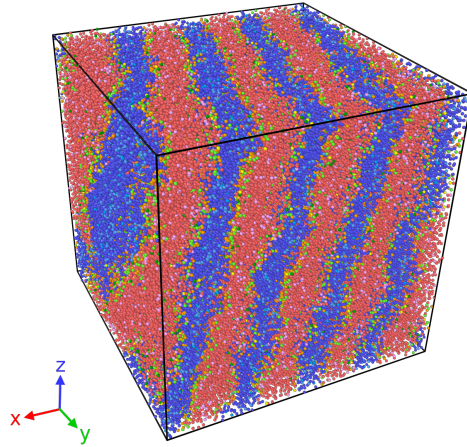


FIG. 8. Lamellar microstructure obtained from a simulation of the blend Miraspec UB75 with composition reported in Table I. The color coding of the beads is shown in Fig. 2 and Fig. 3.

430 B. Miraspec UB75 blend: pressure drops in Sulzer SMX

431 1. Multiscale approach and GPR

432 Once the performance of the DPD model for Miraspec UB75, described in detail in Section II C,
433 was assessed, it was then used to simulate a more realistic macroscopic application. The produc-
434 tion of this blend requires the usage of a static mixer, in which the components are mixed in
435 multiple steps at various temperatures. The multiscale approach is here applied to a simplified
436 version of the production process, isothermal and with uniform composition. The latter is a strong
437 assumption, equal to having the blend already mixed at the entrance of the equipment. Besides
438 the general performances of the multiscale approach, the macroscopic variable of interest is the
439 pressure drop across the mixer.

440 Table X summarize the CFD simulations performed, using an incremental Roman number ev-
441 ery time that an updated GPR model is used. As it is possible to see from this table, three CFD
442 simulations were issued before the whole approach could reach convergence. The criterion here
443 described refers to what, in the multiscale approach, is called *outer loop*, as expressed in Sec-
444 tion III F. To evaluate the convergence of the iterative process, the strain rate interval extracted
445 from a CFD simulation was compared with the one extracted from the previous simulation. The

TABLE X. Maximum and minimum value of the strain rate $\dot{\gamma}$ inside the CFD domain with the different viscosity models. The variable ε is the difference, calculated as relative difference, between the values of one CFD run and the previous.

CFD run	$\dot{\gamma}_{\min} \times 10^{-2} (\text{s}^{-1})$	$\varepsilon_{\min, \text{rel}}$	$\dot{\gamma}_{\max} (\text{s}^{-1})$	$\varepsilon_{\max, \text{rel}}$
Newtonian	3.606		324.98	
GPR I	2.513	0.303	432.30	0.330
GPR II	2.488	0.010	361.05	-0.165

446 convergence criterion is set on the maximum ($\dot{\gamma}_{\max}$) and on the minimum ($\dot{\gamma}_{\min}$) values of the strain
 447 rate intervals, as follows:

$$\varepsilon_{\min, \text{rel}} = \frac{\dot{\gamma}_{\min}^{(n-1)} - \dot{\gamma}_{\min}^{(n)}}{\dot{\gamma}_{\min}^{(n-1)}} \leq 0.01, \quad (17a)$$

448

$$\varepsilon_{\max, \text{rel}} = \frac{\dot{\gamma}_{\max}^{(n)} - \dot{\gamma}_{\max}^{(n-1)}}{\dot{\gamma}_{\max}^{(n-1)}} \leq 0.01, \quad (17b)$$

449 where the superscript (n) refers to the latest CFD simulation and the superscript (n - 1) refers to
 450 the previous CFD simulation. If the strain rate interval of the last CFD simulation is wider than
 451 1% with respect to the one from the previous simulation, the GPR should test the training data on
 452 the newly extracted interval. One should notice that the condition is tested separately for the upper
 453 limit and the lower limit, and both need to be satisfied for convergence.

454 Fig. 9 shows the regression process applied to the first shear rate interval, which is extracted
 455 from the CFD simulation with the Newtonian viscosity model. Besides the rheograms, Fig. 9
 456 depicts also information about the quality of the regression for the GPR loop, called *inner loop*
 457 in the multiscale approach (Section II F). As it is possible to see from Fig. 9.a2 and Fig. 9.b2, to
 458 reach the convergence of the GPR, the following equation must be satisfied in the whole strain rate
 459 interval:

$$\sigma \leq \sigma_{\text{lim}} = 10^{-2} \quad (18)$$

460 with σ_{lim} corresponding to the dotted orange line in the plots. Fig. 9.a1 and Fig. 9.a2 report the
 461 results of an incomplete GPR viscosity model, obtained with a partial training data set of two
 462 ($\dot{\gamma}, \mu(\dot{\gamma})$) couple of points. Fig. 9.b1 and Fig. 9.b2, instead, illustrate the viscosity model GPR I
 463 (Table X), obtained after the convergence of the GPR on the interval extracted from the Newtonian
 464 CFD simulation. Comparing Fig. 9.a1 and Fig. 9.b1 it is possible to illustrate how the addition of

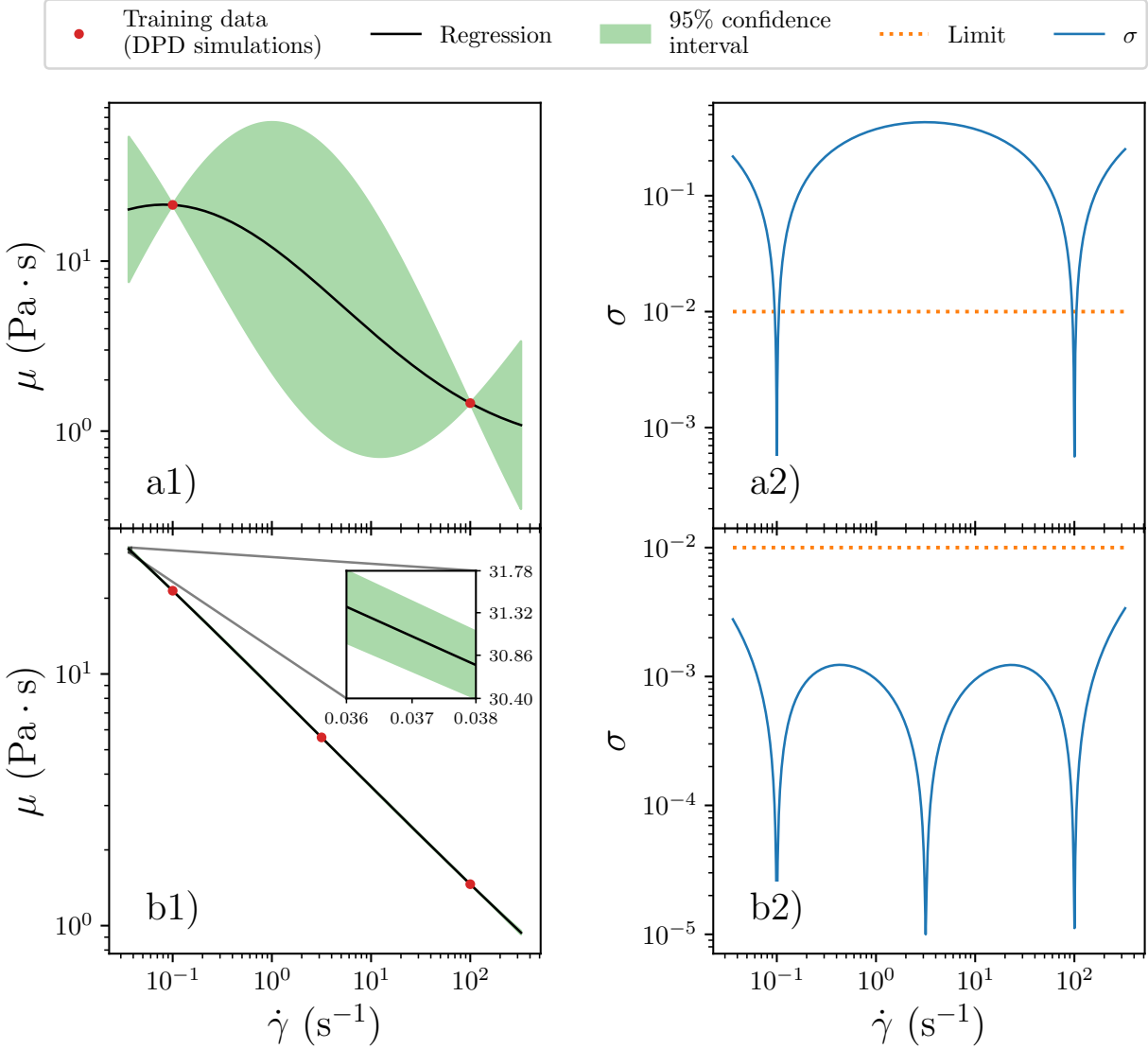


FIG. 9. Illustration of the regression process to build the viscosity model GPR I, using the shear rate interval extracted from the Newtonian CFD simulation. The different plots show: a1) rheogram of the incomplete GPR I model before convergence, a2) standard deviation associated to the regression of the incomplete GPR I model before convergence, b1) rheogram of the converged GPR I model, b2) standard deviation associated to regression of the converged GPR I model. The inset in b1) contains the magnification of a portion of the regression, to allow the visualization of the narrow 95% confidence interval.

465 the third data point to the data set substantially improves the regression. This is confirmed by the
 466 low values of σ shown in Fig. 9.b2, which correspond to a very narrow 95% confidence interval
 467 in Fig. 9.a2, as visible only in the magnified inset.

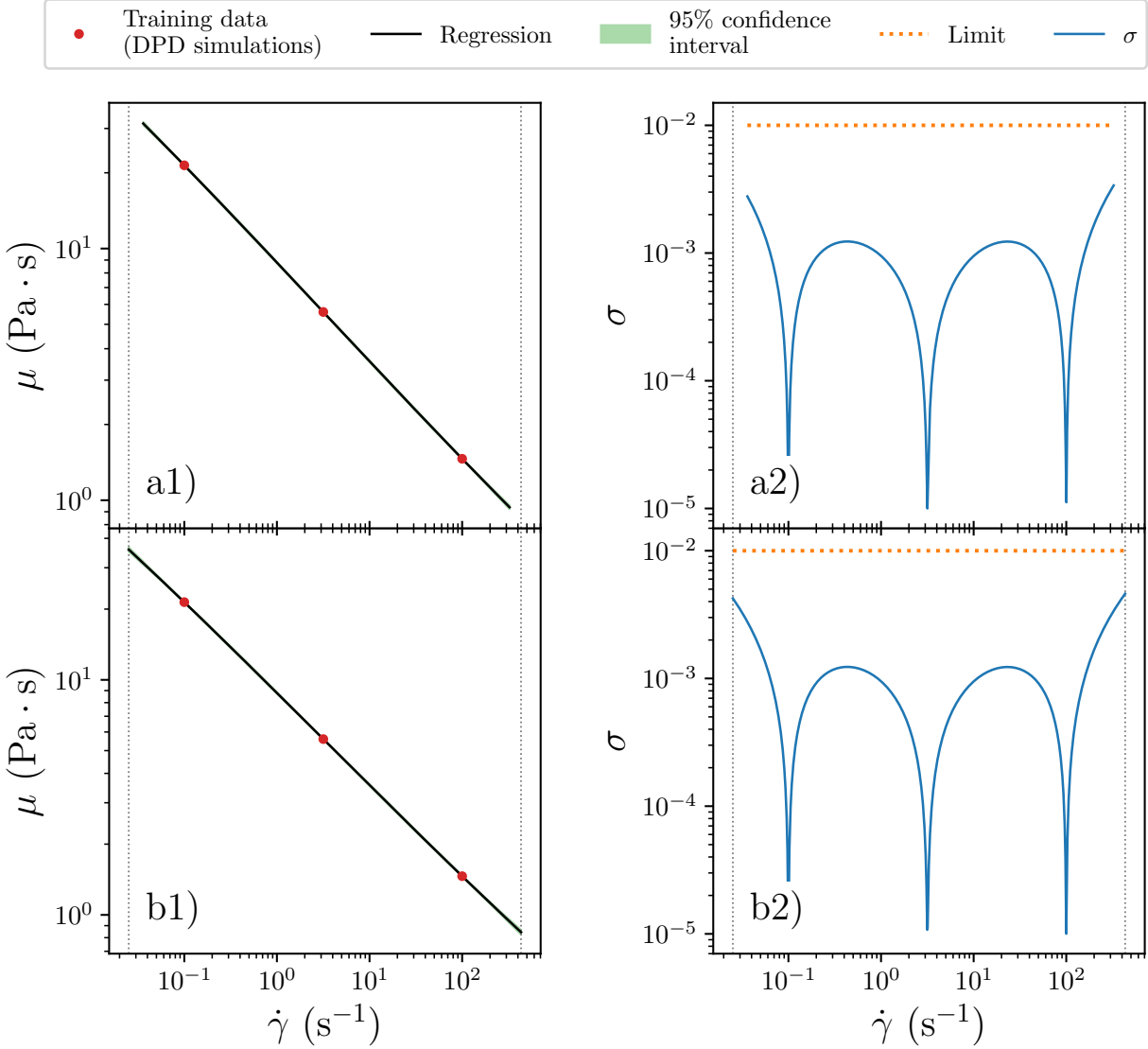


FIG. 10. Comparison between GPR I and GPR II viscosity model. The plots show: a1) rheogram of the converged GPR I model, a2) standard deviation associated to the regression of the converged GPR I model, b1) converged GPR II model, b2) standard deviation associated to the regression of the converged GPR II model. The 95% confidence intervals in a1) and b1) are slightly visible only close the the extremes of the curves, due to their narrowness. The dotted grey vertical lines highlight the different width between the intervals used for the regression in the two models.

468 The GPR I and GPR II viscosity models (Table X) are depicted in figure Fig. 10.a and Fig. 10.b
 469 respectively. As previously stated, the GPR I model is built on the shear rate interval extracted
 470 from the first CFD simulation, which employed a Newtonian viscosity model. The GPR II model

471 is instead built on the shear rate interval extracted from the second CFD simulation, which imple-
 472 mented the GPR I model. Moreover, the training data set used is the same for the two viscosity
 473 models, indicating that no additional DPD simulations were necessary to reach the convergence
 474 of the regression step. Consequently, the two viscosity models are very similar and the only
 475 difference resides in the shear rate interval. Indeed, the GPR II is built on a wider interval, as
 476 emphasized by the dotted vertical grey lines in Fig. 10. The 95% confidence intervals in Fig. 10.a1
 477 and Fig. 10.b1 are very narrow and slightly visible only close to the extremes of the intervals.
 478 Hence, σ reaches its maxima in correspondence to the interval extremes in both Fig. 10.a2 and
 479 Fig. 10.b2, since the GPR technique performs worse in extrapolating than in interpolating. A third
 480 GPR viscosity model was not built since, as reported in Table X, the difference between the last
 481 $\dot{\gamma}$ interval and the previous one respected the convergence criteria in Eq. (17). The difference
 482 between the limits of the strain rate intervals is also noticeable in Fig. 11, where the cumulative
 483 distribution functions of $\dot{\gamma}$ are plotted. The same figure also shows that the $\dot{\gamma}$ distributions for the
 484 two GPR models are basically superimposed, and the differences with the Newtonian one are not
 485 so relevant. The reason for such small differences is probably due to the viscosity value ν used for
 486 the Newtonian simulation. The initial guess for the value of ν resulted to be intermediate when
 487 compared with the extreme values of the final viscosity interval (Fig. 14.a). This could explain
 488 both the slight shift to higher $\dot{\gamma}$ values of the Newtonian distribution and the different shape for
 489 intermediate values of strain rate.

490 A total of three DPD simulations were necessary during the whole process, to have the Eq. (18)
 491 respected, as illustrated by the series labeled as “Training data” in Fig. 9 and Fig. 10. The final
 492 viscosity model obtained with the multiscale approach is of a shear-thinning fluid. This is consis-
 493 tent with the experimental measures available, that usually lead to a power-law viscosity model
 494 for simulation purposes.

495 2. CFD simulations

496 The results of the CFD simulations are analyzed qualitatively through contour plots on the slice
 497 shown in Fig. 12. In this figure, it is reported the Slice \mathcal{A} , that cuts the domain with the plane
 498 $x = 0$ m from the inlet section to the outlet one. In Fig. 13 the just described slice is used to
 499 compare the strain rate $\dot{\gamma}$ inside the domain from different simulations. In these contour plots, it
 500 is shown that the strain rate trend in the domain is similar regardless of the viscosity model used.

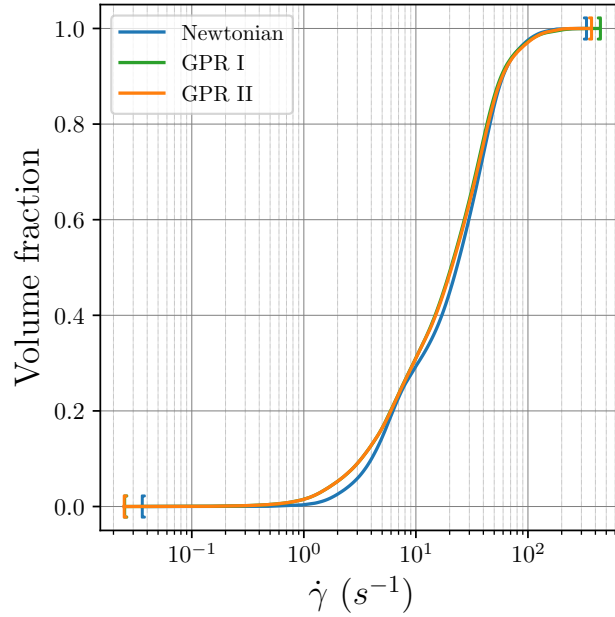


FIG. 11. Volume cumulative distribution function for the shear rate values in the different CFD simulations. The “[” and “]” markers correspond to the $\dot{\gamma}_{\min}$ and $\dot{\gamma}_{\max}$ respectively, for every interval.

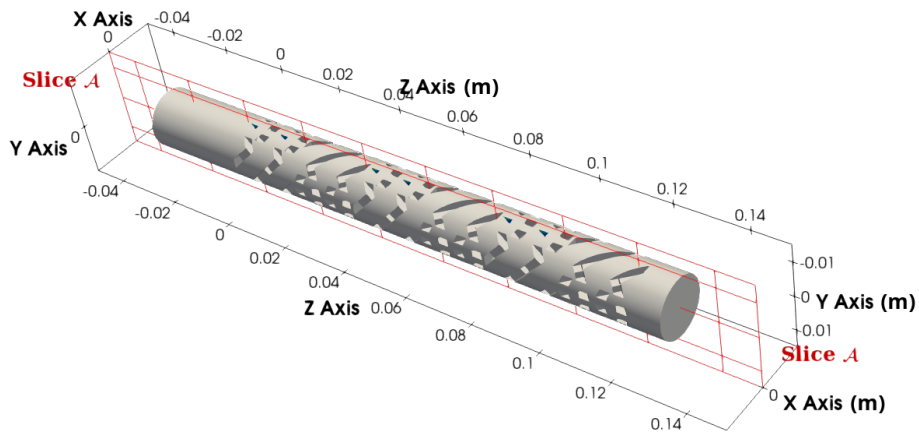


FIG. 12. Visual representation of the slice \mathcal{A} used for contour plots. This cuts the CFD domain with the plane $x = 0$ m. All the lengths in the figure are expressed in meters.

501 The strain rate values are higher close to the walls of the tube and close to the mixing elements,
 502 while regions of low strain rates are found mostly at the inlet and outlet. Hence, the contour for the

503 $\dot{\gamma}$ is in a qualitative agreement with the theory since a steeper variation of the velocity of the fluid
 504 is expected in correspondence with the walls. The only visible differences in the contour plots
 505 are confined to the inlet region in the simulation with the Newtonian model. This is due to the
 506 viscosity value of the fluid in that region, lower than the one in the non-Newtonian simulations,
 507 which consequently influences the distribution of $\dot{\gamma}$

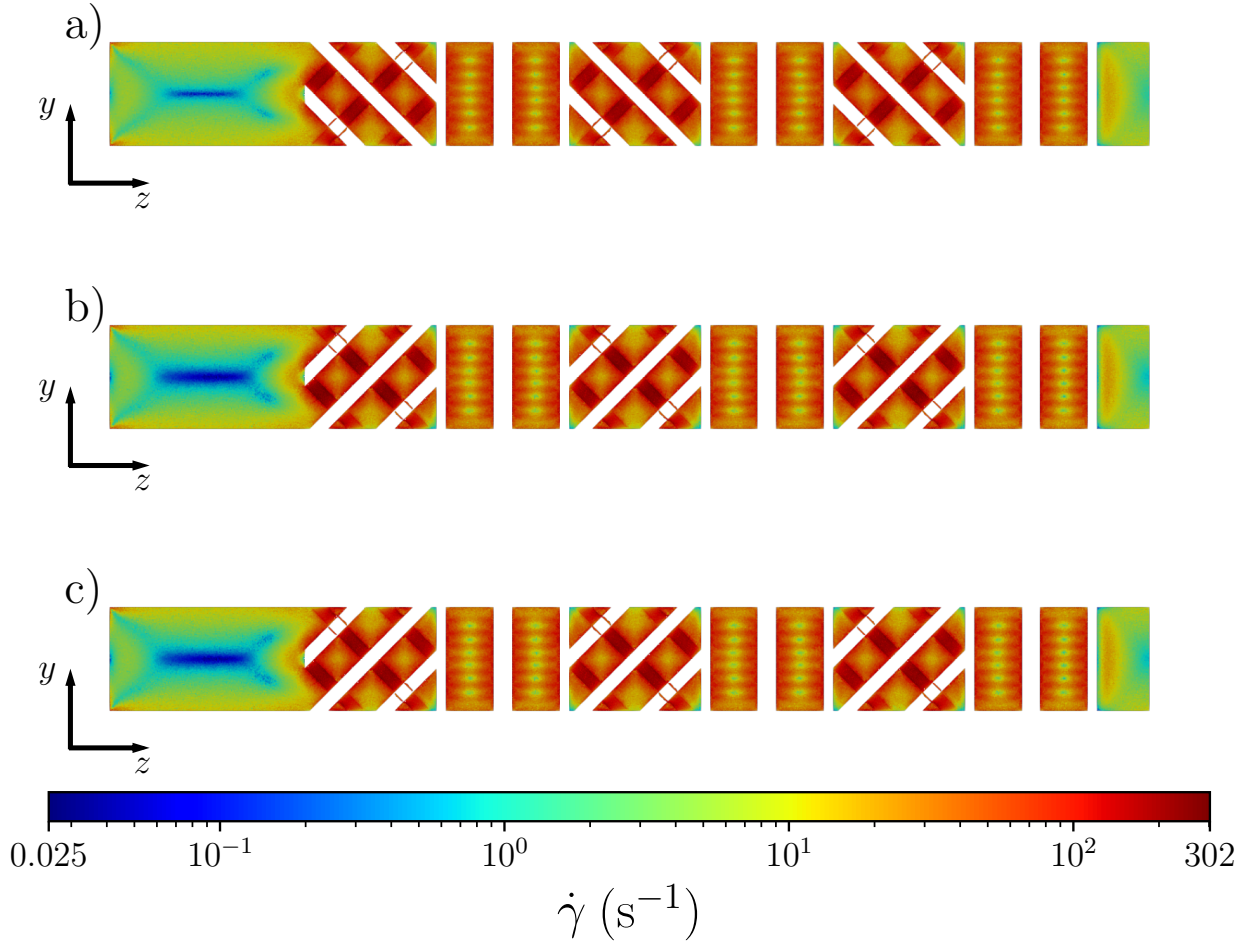


FIG. 13. Contour plot for the strain rate $\dot{\gamma}$ in correspondence of the slice \mathcal{A} . The values are plotted using a logarithmic scale for the colorbar. Different CFD runs are shown: a) Newtonian model, b) GPR I viscosity model, c) GPR II viscosity model.

508 In general, contour plots with similar trends were already obtained as a result of simulations of
 509 different blends with this computational domain. Fig. 14 illustrates the contour plot for viscosity
 510 in the same plane. Since the Newtonian model was employed, Fig. 14.a reports a constant value,
 511 and the viscosity corresponds to an intermediate value when compared to the whole interval of μ

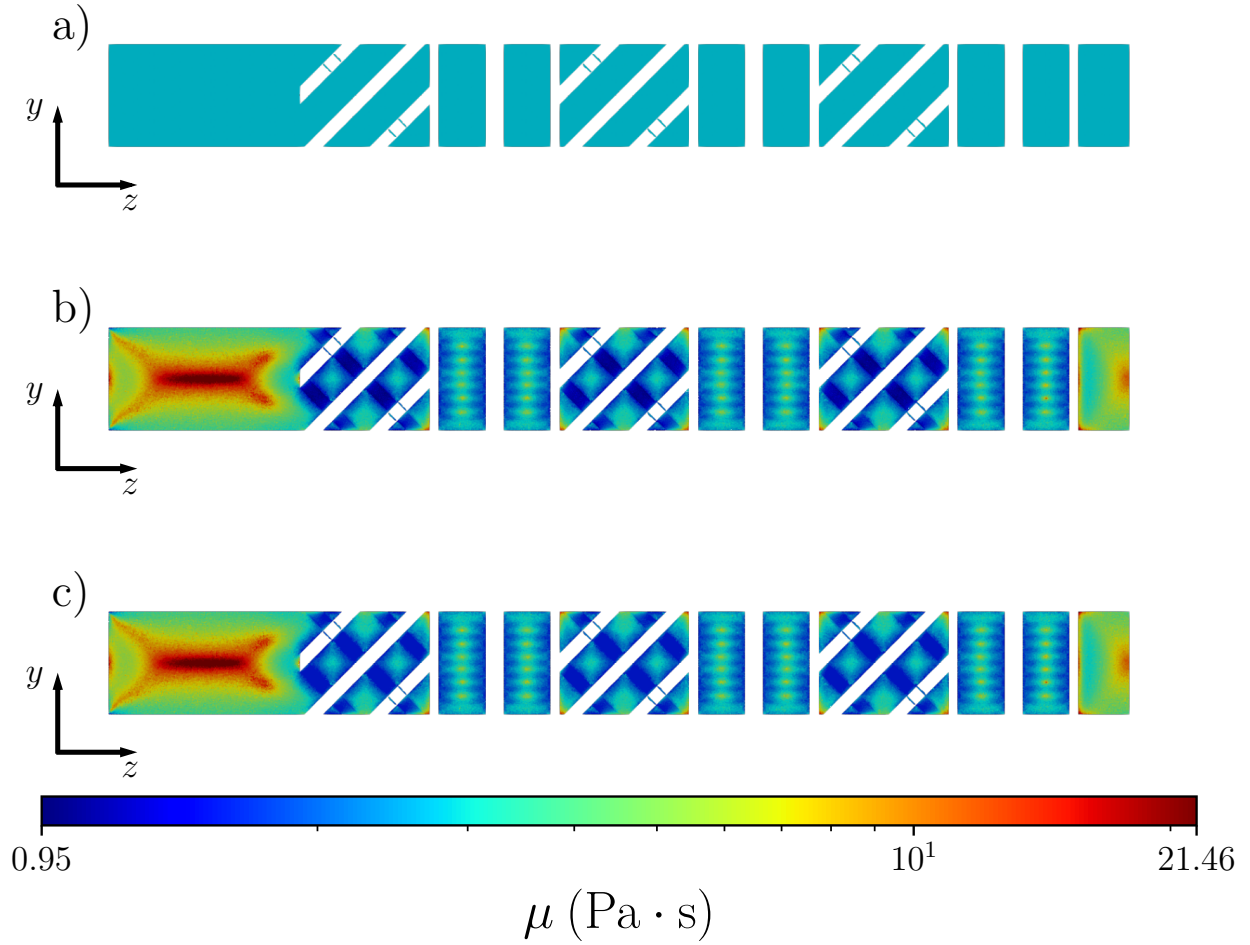


FIG. 14. Contour plot for the viscosity μ in correspondence of the slice \mathcal{A} . The values are plotted using a logarithmic scale for the colorbar. Different CFD runs are shown: a) Newtonian model, b) GPR I viscosity model, c) GPR II viscosity model.

512 explored by the GPR models. As already noticeable from the rheogram in Fig. 10, the model of a
 513 shear-thinning fluid resulted from the DPD simulations. This shear-thinning behavior is visible in
 514 Fig. 14.b, where the viscosity is lower in correspondence with the high strain rate regions of the
 515 mixing elements (Fig. 13.b).

516 When compared with the viscosity of the GPR model, the value of μ for the Newtonian sim-
 517 ulation resulted lower in the inlet and outlet regions, but higher in the mixing section. Since the
 518 latter brings a substantially higher contribution to the pressure drop, the Newtonian model pre-
 519 sented a value of Δp higher by one order of magnitude than the GPR models, as in Table XI.
 520 The difference between GPR I and GPR II can be ascribed to the different $\dot{\gamma}$ explored: the GPR

TABLE XI. Pressure drop across the static mixer system for the different CFD simulations.

CFD run	Δp (Pa)
Newtonian	2.90×10^5
GPR I	2.41×10^4
GPR II	2.50×10^4

521 I simulation reached higher values of strain rate (Table X), resulting in a lower viscosity in the
 522 mixing section and slightly lower Δp . As the final result, the pressure drop obtained from the
 523 last CFD simulation was $\Delta p = 2.50 \times 10^4$ Pa. Though it is not possible to carry a validation of
 524 this result, its order of magnitude can be considered reasonable given the investigations done by
 525 Solvay in static mixers. In particular, a comparison can be done with a mixture at 65% of SLES in
 526 water, flowing in an SMX static mixer with a smaller diameter of 4.95×10^{-3} m. This system has
 527 been studied through CFD simulations and with the correlations proposed by Liu, Hrymak, and
 528 Wood³⁴, using a power law to model its rheology. For a generalized Metzner – Reed Reynolds
 529 number^{34,54} of $Re_{MR} = 6.54 \times 10^{-2}$ it was obtained $\Delta p = 1.66 \times 10^4$ Pa · s from the CFD simu-
 530 lations, and $\Delta p = 1.70 \times 10^4$ Pa · s using the correlation of Liu, Hrymak, and Wood³⁴. By fitting
 531 the experimental measures available on Miraspec UB75 (see Section III B 3 with a power law,
 532 it was possible to calculate $Re_{MR} = 6.38 \times 10^{-2}$ for the simulation of this work. The compar-
 533 isons between these results show an agreement on the order of magnitude, though they cannot be
 534 considered as a validation process.

535 3. Viscosity model from DPD simulations

536 The application of a shear to a DPD fluid still presents some unsolved issues. In particular,
 537 an unphysical shear-thickening behaviour was found even for Newtonian fluids in high shear rate
 538 conditions²². Moreover, for very low shear rate values the thermal noise prevails on the streaming
 539 velocity imposed by the box deformation. As a consequence, it becomes impossible to obtain a
 540 linear velocity profile, *i. e.* a constant imposed shear rate, and apply Eq. (10). The use of DPD
 541 simulations in large shear rate intervals should be tested, to avoid the occurrence of the described
 542 computational artifacts. In this work, partial mitigation of these effects was obtained through
 543 the use of a higher dissipative DPD constant γ combined with the SLLOD equation of motion.

544 Therefore, the results used to build the rheology model were obtained from simulations performed
 545 in a safe DPD shear rate interval.

546 The viscosity results obtained from the DPD simulations were compared with the results of
 547 two sets of experiments, previously performed at Solvay with the blend Miraspec UB75. The
 548 measurements were carried out with the Brookfield DV-II+ viscometer, using the LV3 spindle at
 549 25 °C. The results are shown in Fig. 15, where it is important to remember that the first DPD point
 550 corresponds perfectly because this point was used to identify the conversion factor in Table VI. The
 551 agreement between the simulations and the experiments is remarkably good, but more simulations
 552 and experiments are needed to increase the robustness of the model. In particular, the effect of the
 553 temperature and composition should be taken into account since they can have a great impact on
 554 the value of viscosity of these kinds of mixtures.

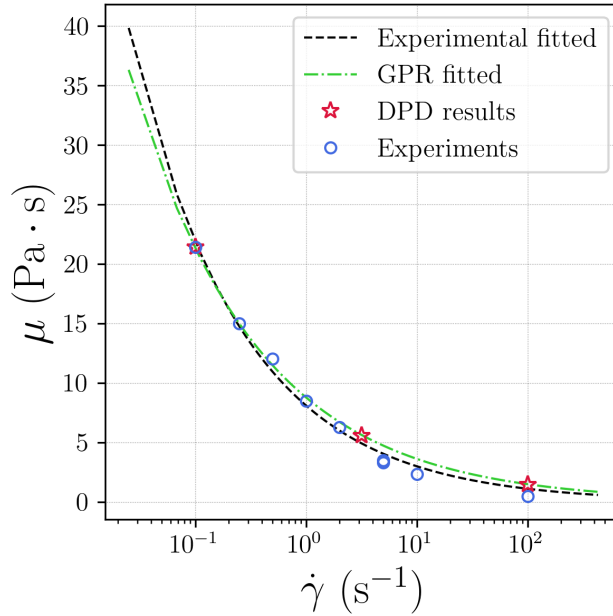


FIG. 15. Comparison between the viscosity model obtained from experimental results and DPD simulations. The blue hollow circles represent the experiments performed at Solvay, and the red hollow stars are the results of the DPD simulations. The black dashed line is the power law resulting from the fitting of the experimental data, while the green dashed and dotted line is the power law resulting from the fitting of one thousand GPR predictions logarithmically spaced on the interval from GPR I in Table X.

555 To further assess the quality of the viscosity model built on the DPD simulations, a power law,
 556 as in Eq. (19), was used to fit both the experimental data and the prediction from the GPR.

$$\mu = m \cdot \dot{\gamma}^{n-1} \quad (19)$$

557 The power law is one of the most commonly used functions in rheology to approximate the be-
558 haviour of shear-thinning fluids for intermediate shear rates. It must be reminded that the GPR
559 does not output a functional form, but a value of apparent viscosity for every value shear rate
560 value in input. Hence, to obtain a power law model for comparison, the GPR was performed to
561 produce one thousand of $(\dot{\gamma}, \mu)$ couple of points in the final interval (GPR I in Table X). These
562 points are fitted with a power law and the comparison with the power law generated from the
563 experimental data is illustrated in Fig. 15, while the parameters of the power law are reported in
564 Table XII. As it is possible to see from Fig. 15 and Table XII, the two fitted functions are close to
565 each other, indicating that the GPR model provides a physically reasonable description.

TABLE XII. Parameters obtained from the fitting process of the experimental and GPR data using the power law in Eq. (19).

Data set	m , (Pa · s ⁿ)	$n - 1$
Experimental	$8.11 \pm 3.0 \times 10^{-1}$	$-0.432 \pm 2.0 \times 10^{-2}$
GPR	$8.81 \pm 3.0 \times 10^{-3}$	$-0.383 \pm 1.4 \times 10^{-4}$

566 4. *Multiscale approach computational performance*

567 The idea behind the approach described in this work is the automatic selection of which DPD
568 simulation to perform. This should lead to a reduction of the computational resources needed,
569 through the minimization of the number of DPD simulations. The simulations were performed
570 on a workstation with a CPU “Intel® Xeon® Gold 6248 CPU @ 3.00GHz” using 24 cores. The
571 time requested by each simulation is reported in Table XIII. Here the CFD simulations are identi-
572 fied through the viscosity model used to perform them, while the DPD simulations are numbered
573 following the order of execution. It is possible to discriminate between these DPD simulations
574 through the applied shear rate, as reported in Table XIV. In Table XIII is, instead, evident that the
575 DPD simulations are the bottleneck of the automated approach, requesting from six to ten times
576 the time of a CFD simulation.

577 For what concerns the variability of the time needed to complete a simulation, it looks that a
578 simulation with the GPR model can take up to four times more time than a Newtonian one. Actu-
579 ally, the Newtonian simulation stopped after 588 iterations, while the GPR model continued until

TABLE XIII. List of simulations in the order in which they were performed, with the corresponding computational time. The performed *inner loops* are also indicated.

	Simulation	Computational time (h:m)
1° GPR–DPD loop	CFD Newtonian	0:14
	DPD 1°	6:08
	DPD 2°	11:24
	DPD 3°	8:02
	CFD GPR I	1:09
	CFD GPR II	1:10

580 2000 iterations. This can be the sign of too strict convergence criteria for the CFD simulation,
 581 which can be affected not only by the viscosity model but also by the quality of the mesh. Conse-
 582 quently, a different mesh or a better choice of the convergence parameter could lead to a reduction
 583 of the computational time.

TABLE XIV. List of DPD simulations with the corresponding time to completion and the imposed shear rate $\dot{\gamma}$. The simulations are ordered with increasing $\dot{\gamma}$, to highlight the dependence of the requested time on the imposed shear rate.

Simulation	$\dot{\gamma}$ (DPD units)	Computational time (h:m)
DPD 1°	0.01	6:08
DPD 3°	0.317	8:02
DPD 2°	10	11:24

584 Conversely, for the DPD simulation, there is a strong dependence of the computational time
 585 on the value of $\dot{\gamma}$. Higher values of the shear rate imposed on the simulation box lead to longer
 586 computational times to complete the simulation, according to Table XIII.

587 Using an automated approach for choosing the best shear rate value to add a point to the training
 588 data set led to satisfactory results in terms of computational time. Nonetheless, it must be noted
 589 that the rheogram resulted simple enough to obtain a good quality regression with only three
 590 training points. Consequently, to assess the computational advantages of this approach with more
 591 accuracy, it should be tested on a more complex rheology model, *e.g.* including the effect of

592 composition. Instead, for what concerns the CFD and DPD techniques, the computational time
593 depends strongly on the models implemented in these kinds of simulations, so it is not possible to
594 make a generalization.

595 **IV. CONCLUSIONS**

596 The main purpose of the work was to develop a multiscale automated approach that could allow
597 the simulation of fluids in a typical mixing piece of equipment. The macroscale Computational
598 Fluid Dynamics (CFD) simulations are used to get information on macroscopic variables, such
599 as the pressure drops across a static mixer. The mesoscale Dissipative Particle Dynamics (DPD)
600 simulations are instead used to build a rheology model for the non-Newtonian fluid of interest.
601 In order to reduce the computational resources needed for the simulations, the Gaussian Process
602 Regression (GPR) was used to build the rheological model from the DPD non-equilibrium simu-
603 lations.

604 The fluid of interest, the blend Miraspec UB75, was modelled using a parametrization devel-
605 oped for similar surfactants. Using this parametrization, a part of the phase diagram of a mixture
606 of SLES and water was successfully reproduced from a qualitative point of view. This confirmed
607 the capabilities of the DPD technique to obtain qualitative information about the microstructure
608 of the simulated fluids. Non-equilibrium simulations were used to reproduce the rheological be-
609 haviour of the fluid under the application of shear stress. The application of the shear condition on
610 the simulation box showed some limitations of the DPD method, regarding the explorable shear
611 rates. It was noticed that for too high or too low values of $\dot{\gamma}$, the results of the non-equilibrium
612 simulations are less reliable. This is common to all atomistic methods, but it would be beneficial
613 to study how to mitigate the effects of extreme strain rate conditions on the quality of the pre-
614 dictions. Despite this issue, it was possible to reproduce the rheological behaviour of the studied
615 fluid. The obtained Δp were realistic when compared to the behavior of similar blends in the same
616 mixing devices. Moreover, the value of viscosity obtained with the DPD simulation resulted in
617 remarkably good agreement with two sets of experiments conducted at different shear rates. This
618 is noteworthy in light of the approach used for the identification of the conversion factors, which
619 is often a weak point in non-equilibrium DPD simulations. Indeed, deriving the conversion factor
620 by matching the value of viscosity for the lowest applicable shear rate led to promising results.

621 To conclude, this work shows the feasibility of an automated multiscale approach to describe a

622 real system that is relatively simple in terms of chemical composition, but further studies should
623 be conducted to explore the limits of the DPD technique. Among these, the more critical are
624 the parametrization of the molecules and the description of local charges, the width of the ex-
625 plorable shear rate interval in non-equilibrium simulations, and the possibility of simulation for
626 non-isothermal systems. Furthermore, an experimental campaign could allow a more robust vali-
627 dation of the developed model.

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638

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