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# Reactive fluid flow topology optimization with the multi-relaxation time lattice Boltzmann method and a level-set function

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1     Reactive fluid flow topology optimization with the  
2     multi-relaxation time lattice Boltzmann method and a  
3                     level-set function

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11    **Abstract**

This paper presents a topology optimization algorithm based on the lattice Boltzmann method coupled with a level-set method for increasing the efficiency of reactive fluid flows. The multi-relaxation time model is considered for the lattice Boltzmann collision operator, allowing higher Reynolds numbers flow simulations compared to the ordinary single-relaxation time model. The cost function gradient is obtained with the derivation of the adjoint-state formulation for the fully coupled problem. The proposed method is tested successfully on several numerical applications involving Reynolds numbers from 10 up to 1,000, as well as with different Damkohler and Peclet numbers. A limitation of the maximal pressure drop is also applied. The obtained results demonstrate that the proposed numerical method is robust and efficient for solving topology optimization problems of reactive fluid flows, in different operating conditions.

12    *Keywords:* Topology optimization, adjoint-state formulation, reactive fluid  
13    flow, lattice Boltzmann method, level-set method

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## 14 1. Introduction

15 The development of efficient reactors is needed in many chemical pro-  
16 cess and energy applications: chemical synthesis, catalytic combustion, and  
17 electro-chemical conversion, to cite but a few. The growth of renewable en-  
18 ergy (wind, solar, or marine) implies an improvement of the electricity storage  
19 technologies. Electrolysers, or redox-flow batteries, can be used for the first  
20 stage of the electro-chemical conversion, and fuel cells for the reverse reac-  
21 tions. One of the principal characteristics to improve is the power density  
22 ( $\text{kW}/\text{m}^3$ ,  $\text{kW}/\text{m}^2$  or  $\text{kW}/\text{kg}$ ) that represents the "good use" of the consti-  
23 tutive materials. All these systems can be seen as electrochemical reactors,  
24 where reactants are supplied to the reaction place by convection and diffusion  
25 mechanisms while by-products (thermal energy or new species) need to be  
26 removed (to avoid thermal problems or to leave free access to the reaction  
27 location). In the case of conventional vanadium redox-flow batteries, the re-  
28 action occurs on the material surface, whereas in the case of fuel cells, the  
29 species transport is more complicated. For example, in the case of polymer  
30 exchange membrane fuel cells (PEMFC), the reactants are usually trans-  
31 ported into the gas channels and are diffused through a thin porous medium,  
32 in order to reach the catalyst layers (anode or cathode).

33 In this context, the efficiency of the reaction depends on the fluid flow  
34 channels geometry inside the domain. Some geometries have been tested in  
35 literature to this matter (serpentine [1], inter-digitated [2], etc.), but there  
36 are still discussions about which configuration is optimal, or the best, and  
37 benchmark parameters are not well-established [3]. Structural optimization  
38 techniques provide a promising method to overcome the strong limitation of  
39 determining *a priori* a system's geometry. Previous methods required this  
40 to be specified to allow optimization through testing relevant parameters  
41 (e.g. channel dimensions), significantly limiting the structural configurations  
42 possible.

43 Doing so, the fluid/solid distribution is to be determined via optimiza-  
44 tion methods. Among the three main optimization methods, namely the  
45 size optimization, the shape optimization, and the topology optimization [4],  
46 the latest is associated to the highest number of degrees of freedom. With  
47 topology optimization, very different geometries can be dealt with and ob-  
48 tained, leading to high levels of geometrical complexity, and with the ability  
49 of creating holes inside the domain of interest (this is not possible with either  
50 optimization strategies of size and shape optimization).

51 The basic idea of topology optimization is to optimize a material alloca-  
52 tion problem where the material can have different properties. One of the  
53 first applications concerns the structural mechanical optimization, with com-  
54 pliance minimization [5, 6]. In that case, the material is either void or solid,  
55 but it can also be fluid or solid, in order to build fluid channels, for example.  
56 Topology optimization is well developed for fluid flow designs [7–10], but  
57 most often for solving pressure drop minimization problems.

58 One challenge of topology optimization is to develop multi-physics ap-  
59 plications. As the complexity of the physics increases for these problems,  
60 topology optimization can be helpful to suggest innovative geometries that  
61 could not be intuitively thought. Although some topology optimization algo-  
62 rithms have been proposed for some heat transfer applications [11–15], the  
63 development of such methods for chemical reaction is relatively scarce. Non  
64 exhaustively, the following works are of great interest. In their seminal pub-  
65 lication, Okkels et al. [16] extended the work of Borrvall et al. [7] in the case  
66 of advection-diffusion-reaction problem. They worked on a catalytic micro-  
67 reactor for topology optimization and compared their results with empirical  
68 geometries, like a uniform or a membrane reactor. They also studied the  
69 influence of the relevant physical parameters on the optimized geometries.  
70 Schäpper et al. [17] dealt with topology optimization of bio reactors. They  
71 could show that the production of protein could be improved with topology  
72 optimization compared to a conventional reactor with a uniform distribution  
73 of biomass. A compromise is found for the glucose flowrate, sufficient enough  
74 for the reaction to happen and limited to avoid a strong ethanol production,  
75 which decreases the enzym activity. Yaji et al. [18] worked on vanadium  
76 redox flow batteries to provide a sufficient supply of species to the carbon  
77 fiber electrode, under a pressure drop constraint. The electrode is modeled  
78 as a porous medium with Darcy’s law and the generation rate depends on  
79 the local velocity. The resulting optimal structure is an interdigitated flow  
80 field with strong tortuosity. This is due to the porous structure of the solid  
81 electrode, encouraging the flow through it in order to enhance the reaction.  
82 Kim et al. [19] worked on PEM fuel cells optimization in order to maximize  
83 the reaction rate between hydrogen and oxygen. Their topology optimization  
84 method has been applied to different geometry initializations such as centered  
85 inlet and outlet, multi-terminal inlet and outlet or serpentine channels.

86 In these three studies: [16–18], the catalyst for the reaction is located di-  
87 rectly on the porous support, whereas in [19], the reaction takes place in the  
88 fluid channels. In this last application, the specificity of a PEM fuel cell with

89 different layers is taking into account: the optimization deals with the best  
90 way to feed reactant into a planar electrode and the solid has two functions:  
91 electrode supporting and fluid routing. The work presented in this article  
92 will follow the same approach. All the previously cited works rely on the  
93 SIMP modelization regarding the design material. This one is represented  
94 by a scalar field varying continuously from 0 (solid) to 1 (fluid). Intermediate  
95 states are penalized during the optimization process in order to promote a  
96 clear transition between the solid and the fluid. However, gray-scale effects  
97 occur, and, as mentioned by Makhija et al. [20], the porosity model does  
98 not prevent diffusion into and through solid regions, excluding low Peclet  
99 number simulations, when advection and diffusion are of the same order of  
100 magnitude. In order to overcome this issue, a level-set function (LSF) was  
101 used in this study for the fluid/solid representation. As the level-set function  
102 is continuous, it provides a continuous fluid/solid transition as required by  
103 the optimization process. However it is possible to use the zero contour of  
104 the LSF in order to get a clear fluid/solid interface. This latter feature is  
105 particularly interesting to obtain accurate boundaries for the forward prob-  
106 lem. Many different methods can fall under a level-set appellation. Differing  
107 from the original work of Allaire [21], the evolution of the level-set function  
108 will not be realized with the Hamilton-Jacobi equation combined with shape  
109 derivatives. A similar approach to that of Yamada [22] was applied here,  
110 with no advection in the LSF evolution equation but only a source term de-  
111 pending on the design sensitivities. With this method, the LSF does not need  
112 to be re-initialized during the optimization process and the creation of dis-  
113 continuity in the material distribution is also possible. A smooth Heaviside  
114 function is proposed for the calculation of the cost function gradient, and a  
115 threshold is then applied to compute the forward problem, with discrete 0-1  
116 boundaries.

117 Next, all the works previously cited for the topology optimization of chem-  
118 ical process were based on a finite element strategy to solve both the Navier-  
119 Stokes equations and the advection-diffusion-reaction equation. As an al-  
120 ternative to ordinary discretization methods (finite element method (FEM),  
121 finite volume method (FVM)), the lattice Boltzmann method (LBM) may  
122 be very efficient for solving that kind of problem. Originally, this method  
123 has been used for fluid flow problems [23, 24] in which both the displace-  
124 ment and the collision of particles are solved via the Boltzmann equation,  
125 involving a (often simplified) collision operator. The macroscopic quantities  
126 for the flow field (density, pressure, velocity) can then be recovered by the

127 moments of the distribution function involved in the Boltzmann equation.  
128 Since the pioneering work of Pingen [25], adjoint-state LBM methods have  
129 also been developed for fluid flow identification [26, 27] or topology optimiza-  
130 tion [15, 28, 29]. It is also to be noticed that the LBM computational time  
131 of both forward and adjoint-state problems can be significantly reduced with  
132 GPU parallel computing [30–32]. Further, with the use of a uniform grid,  
133 the remeshing process may not be necessary along with the optimization it-  
134 erations. This is another clear advantage of the LBM over FEM and FVM:  
135 it is indeed very convenient in topology optimization where the complex  
136 fluid/solid geometry evolves with the iterations of the optimization process.  
137 Also, the LBM boundary conditions are easy to implement (bounce-back at  
138 no-slip walls for example) making the LBM a good candidate if fluid/solid  
139 porous structures need to be computed, which can occur in topology opti-  
140 mization with the creation of complex geometries. Generally speaking, the  
141 LBM is convenient for multiphase flows, as the interface can be implicitly  
142 tracked with multiple distribution functions [33]. Though being beyond the  
143 scope of this article, such physics will be used in oncoming research.

144 In order to compute reactive flows, the concentration field is represented  
145 by a passive scalar quantity which is transported by the fluid flow. This  
146 quantity is computed in the LBM framework by a double distribution func-  
147 tion approach [34, 35], more stable than multi-speed models [36]. Another  
148 distribution function is thus introduced to compute this concentration, in  
149 addition to the first distribution function used within the ordinary LBM re-  
150 lated to the fluid flow only. Compared to the previous work done in LBM  
151 topology optimization in thermal fluid flow problems [15], a source term is  
152 introduced in this distribution function to represent the consumption of the  
153 reactant during the chemical reaction. Reaction laws are very numerous  
154 and can be highly nonlinear and multi-parameters dependent (for example  
155 Arrhenius law for the temperature dependence). In optimization literature,  
156 generally, the reactant equation has a linear dependence with the concentra-  
157 tion. At the inlet, the reactant concentration is maximum, before decreasing  
158 inside the domain. The chemical reaction is then considered optimized when  
159 the reactant is fully consumed at the outlet. Mathematically speaking, this  
160 optimization problem consists in minimizing the mean concentration at the  
161 outlet. Obviously, one can seek not only for the full use of the reactant but  
162 also for the best use of reactant: many reaction problems require an homo-  
163 geneous reaction rate, in order to avoid either over heating for exothermic  
164 reactions or catalyst aging. In this case the optimization is multi-objectives

165 (for example searching for an entire consumption of the reactant and an ho-  
166 mogeneous reaction rate at the same time) and requires specific numerical  
167 methods; this problematic is beyond the scope of this publication.

168 In this article, a topology optimization method for an advection-diffusion  
169 reaction problem using the lattice Boltzmann method and a level-set function  
170 is presented. A multiple relaxation time operator is used to compute fluid  
171 flows with Reynolds numbers up to 1,000 and for different Schmidt numbers  
172 (ratio between the momentum diffusion and the mass diffusion) [20]. As this  
173 study depends on several physical parameters (flow regime, reactant mass  
174 diffusivity, reaction rate), their influence on the forward problem and on the  
175 optimized geometry is also investigated. A limitation of the pressure drop is  
176 also introduced in the optimization problem as a constraint.

177 The paper is organized as follows. Section 2 introduces the main features  
178 of the topology optimization method including the update of the geometry  
179 with a level-set function. Section 3 presents the background theory for LBM  
180 and its application for an advection-diffusion reaction equation. This forward  
181 problem is eventually written down concisely in residual form, and the cost  
182 function to be minimized is also rewritten in terms of lattice Boltzmann vari-  
183 ables. Section 4 presents the derivation of the cost function gradient through  
184 the adjoint-state method. The concise residual form is again given. Section 5  
185 then presents the numerical examples related to the topology optimization  
186 of an advection-diffusion reaction problem. The geometry of the problem is  
187 a 2D square cavity with the inlet close to the top-left corner and the outlet  
188 close to the bottom-right corner; the reaction occurs in the entire domain.  
189 This academic test case is a variation of the 2D cavity studied by Okkels  
190 and Bruus [16], but the methodology presented in the current paper can be  
191 extended to real-life applications and 3D configurations. First, a study about  
192 the influence of the Reynolds number is presented with Reynolds numbers  
193 from 10 to 1,000. This range is chosen to explore solutions at sufficiently  
194 high Reynolds numbers to have a benefit in stability with the MRT-LBM  
195 model used here, while focusing on the laminar regime to maintain the valid-  
196 ity of the model. Then the influence of the other physical parameters (Peclet  
197 or Damkholer numbers) is also discussed. All the obtained results demon-  
198 strate that the proposed numerical method is robust and efficient for solving  
199 topology optimization problems of reactive fluid flows, in various operating  
200 conditions. Some discussions and conclusions are finally drawn in section 6.

201 **2. Definition of the optimization problem**

202 *2.1. The physics of advection-diffusion-reaction*

The chemical species are transported by the fluid flow and the reaction is taken into account by a source term involved in the equation of the species concentration. This problem is written with the following macroscopic equations  $\forall \mathbf{x} \in \mathcal{D}$ ,  $\mathcal{D}$  being an open bounded set of  $\mathbb{R}^2$ :

$$\nabla \cdot \mathbf{u} = 0, \quad (1)$$

$$(\mathbf{u} \cdot \nabla) \mathbf{u} + \frac{1}{\rho} \nabla p - \nu \nabla^2 \mathbf{u} = 0, \quad (2)$$

$$\mathbf{u} \cdot \nabla c_A - D \nabla^2 c_A + s = 0. \quad (3)$$

203 The source term  $s$  involved in eq. (3) is expressed as a function of the  
 204 concentration of the species of concern,  $c_A = [A] = \frac{n_A}{V}$ . One possibility is to  
 205 express a linear dependency between  $s$  and  $c_A$ , as in [19]. Elsewhere, in [17]  
 206 and [18], the reaction rate is limited by the ethanol production, or by the  
 207 velocity field, meaning that the reaction rate reaches a maximum value  $k$  for  
 208 a specific concentration. Many other models can be used depending on the  
 209 chemical reactions, using linear, quadratic, cubic, logarithmic, or exponential  
 210 relations, to cite but a few [37, 38]. With a linear source term,  $s = k c_A$ , when  
 211 introducing a given characteristic length of the computational domain  $L$ , and  
 212 a characteristic velocity  $U$  into the initial set of equations eqs. (1) to (3), and  
 213 combining the three physical parameters, namely the fluid viscosity,  $\nu$ , the  
 214 mass diffusivity of the chemical species,  $D$ , and the maximal reaction rate,  
 215  $k$ , one can recover the classical dimensionless version of the initial problem:

$$\tilde{\nabla} \cdot \tilde{\mathbf{u}} = 0, \quad (4)$$

$$(\tilde{\mathbf{u}} \cdot \tilde{\nabla}) \tilde{\mathbf{u}} + \tilde{\nabla} \tilde{p} - \frac{1}{\text{Re}} \tilde{\nabla}^2 \tilde{\mathbf{u}} = 0, \quad (5)$$

$$\tilde{\mathbf{u}} \cdot \tilde{\nabla} \tilde{c}_A - \frac{1}{\text{Pe}} \tilde{\nabla}^2 \tilde{c}_A + \text{Da} \tilde{c}_A = 0. \quad (6)$$

216 Here tilde values  $\tilde{X}$  stand for dimensionless version of  $X$  and the three  
 217 dimensionless numbers Re, Sc and Da are defined as follow:

- 218 • the Reynolds number,  $\text{Re} = \frac{UL}{\nu}$ , represents the ratio between inertial  
 219 and viscous forces involved in a fluid flow. It can help to distinguish  
 220 flow regimes, from laminar to turbulent flows;



- 221 • the Schmidt number,  $Sc = \frac{\nu}{D}$ , is the ratio of the kinematic viscosity  
222 (momentum diffusivity) over the mass diffusivity;
- 223 • the Damkohler number,  $Da = \frac{kL}{U}$ , represents the ratio of the reaction  
224 rate over the transport phenomena rate in the system.

225 Alternatively, the Peclet number can be used,  $Pe = Re \times Sc$ . It represents  
226 the ratio between the transfer by convection and the transfer by diffusion.

227 In fluid flow topology optimization problems, the principal effect of mod-  
228 ifying the topology is the modification of the velocity distribution. It means  
229 that for the optimization to be effective, the convection process has to play a  
230 major role for the concentration distribution when compared to the diffusion  
231 process. Otherwise, the influence of the advection process on the efficiency  
232 of the chemical reaction would be too small. So a high Peclet number is  
233 chosen here to respect this condition. However, diffusion dominant processes  
234 can also be optimized using this method but the problem will be simpler by  
235 removing eqs. (1) to (2) to the set of equations to be solved. About the re-  
236 action rate, a compromise is to be found: if the reaction rate represented by  
237 the Damkohler number is too high, the reactant is consumed too fast in the  
238 domain, and, there is no need of using any topology optimization algorithms.  
239 Completely on the other hand, if the reactant is consumed too slowly, then  
240 the concentration gradients are too small and the impact of the fluid/solid  
241 geometry will also be negligible. For these two extreme cases, the optimiza-  
242 tion problem is insensitive because of the bad sizing of the space domain  $\mathcal{D}$   
243 : this one has to be decreased (resp increased) in order to improve the sensi-  
244 tivity of the physical problem to the topology of the domain. In all cases in  
245 between, for ordinary reaction rates, the use of topology optimization may  
246 be very impact-full.

## 247 2.2. *Setting up the optimization problem: reaction maximization*

248 In topology optimization, one searches for the best material distribution  
249 – or at least a good enough distribution – to satisfy a given objective. The  
250 material distribution is represented by the design variable, and the objective  
251 is defined in terms of a cost function,  $\mathcal{J}$ . The update of the geometry will be  
252 obtained by the evolution of a level-set function, involving the cost function  
253 gradient. This gradient is given by the derivative of the cost function  $\mathcal{J}$  with  
254 respect to the design variable. Section 4 is dedicated to such a derivation.  
255 The objective of the optimization problem is the maximization of the reac-  
256 tion, which is equivalent to the minimization of the product of the velocity

257 with the concentration, at the outlet of the domain. Mathematically, this is  
 258 written as:

$$\mathcal{J} = \frac{1}{|\partial\mathcal{D}_{\text{out}}|} \int_{\partial\mathcal{D}_{\text{out}}} \mathbf{u} \cdot \mathbf{n} c_A + D\nabla c_A \cdot \mathbf{n} \, d\mathbf{x}, \quad (7)$$

259 where  $\mathbf{n}$  is the outward unit normal vector to the boundary, the first term of  
 260 the integral is the convective part of the reactant flux while the second term  
 261 represents the diffusive component. As the Pe number is far greater than one  
 262 in all simulations, the diffusive component is neglected in this work.

263 A constraint is also to be added to the optimization problem in order to  
 264 allow a maximum amount of pressure drop during the optimization process.  
 265 Such a limitation is useful to prevent from unfeasible designs. Rather than  
 266 adding inequality constraints on the optimization problem, a penalization  
 267 term is added to the cost function, as in [39], in structural optimization, for  
 268 example. The augmented cost function,  $\mathcal{J}^+$ , to be minimized, is thus:

$$\mathcal{J}^+ = \mathcal{J} + \ell \mathcal{J}_1 \quad \text{with} \quad \mathcal{J}_1 = \Delta p_{\text{max}} \exp\left(\frac{\Delta p}{\Delta p_{\text{max}}}\right), \quad (8)$$

269 and  $\ell \in \mathbb{R}^+$  is a user-defined value controlling the relative importance of the  
 270 different contributions  $\mathcal{J}$  and  $\mathcal{J}_1$ .

### 271 2.3. Geometry update

272 The design domain is divided into  $N$  elements and there is one design  
 273 parameter per element. The topology is represented by the signed variable  
 274  $\alpha(\mathbf{x}) \in \mathbb{R}^N$ . Then the level-set method is used for the mapping of the design  
 275 variable. Such a method has been firstly implemented for the representa-  
 276 tion of interfaces in multiphase flows [40] and for image segmentation [41].  
 277 It has then been used for topology optimization, by Sethian et al. [42],  
 278 Wang et al. [43], and Allaire et al. [44].

279 The continuous level-set function, is such that its zero contour defines the  
 280 interface between the two media. The update of the solid/fluid distribution  
 281  $\alpha$  is thus performed in two steps. The first one is via the evolution of the  
 282 discrete level-set function  $\Psi(\mathbf{x}) \in \mathbb{R}^N$ :

$$\Psi^{(n+1)}(\mathbf{x}) = \Psi^{(n)}(\mathbf{x}) - \mathbf{P}^{(n)} \nabla_{\Psi} \mathcal{J}^{+(n)}(\mathbf{x}). \quad (9)$$

283 The superscript is the iteration count,  $\mathbf{P}$  is the iteration matrix, ideally  
 284 a good approximation of the inverse of the Hessian matrix,  $\mathbf{P} \approx \widehat{\mathbf{H}}^{-1}$ , and  
 285  $\nabla_{\Psi} \mathcal{J}^+$  is the augmented cost function gradient (this vector contains the

286 derivatives of the cost function with respect to all components of  $\Psi$ ). The  
 287 second step is the topology update which consists in applying the mapping  
 288 between the level-set function and the topology.

289 In a previous study, the mapping from the level set function to the topol-  
 290 ogy was defined as [15]:

$$\alpha(\Psi(\mathbf{x})) = \frac{1}{2} (1 + \text{sign}\Psi(\mathbf{x})), \quad (10)$$

291 such that

$$\alpha(\mathbf{x}) = \begin{cases} 0 & \text{if } \Psi(\mathbf{x}) < 0; \\ 1 & \text{if } \Psi(\mathbf{x}) > 0. \end{cases} \quad (11)$$

292 A smooth version of the mapping can be considered, for example [45]:

$$\alpha_\epsilon(\Psi(\mathbf{x})) = \frac{1}{2} + \frac{1}{\pi} \arctan \frac{\Psi(\mathbf{x})}{\epsilon}. \quad (12)$$

293 The main interest in using (12) rather than (10) is that the former is  
 294 a continuous and differentiable function, with  $\alpha'_\epsilon(\Psi)$  finite everywhere, as  
 295 soon as  $\epsilon \neq 0$ . Besides, if  $\epsilon \rightarrow 0$ , a clear discontinuous fluid/solid interface  
 296 is obtained, which is useful while solving the forward problem. Indeed, the  
 297 LBM implementation used here for the fluid flow and for the concentration  
 298 field does not involve a force term to deal with a Brinkmann penalization for  
 299 a porous media. As a consequence, each node must be either strictly fluid  
 300 or solid, and no intermediate state is allowed. It means that a threshold is  
 301 applied after the update of the level-set function to obtain a clear fluid/solid  
 302 interface for the forward problem. The choice of this parameter  $\epsilon$  is discussed  
 303 in the section dedicated to numerical results. In the following, the subscript  
 304  $\epsilon$  is avoided for readability considerations.

305 Note that other strategies such as the Brinkmann penalization for mod-  
 306 eling the porous medium, coupled with the SIMP method could have been  
 307 used [20]. However, the level-set function allows a clearer definition of the  
 308 topology, and thus minimizes the possible bias involved within the forward  
 309 model.

310 **3. Lattice Boltzmann method**

311 *3.1. Multi-relaxation time model for the fluid flow*

312 The lattice Boltzmann method (LBM) is an alternative way of solving  
 313 fluid flow problems compared to classical methods based on the discretiza-  
 314 tion of the Navier–Stokes equations (finite volume or finite element methods).  
 315 This method is based on the calculation of the distribution function  $f$  in-  
 316 volved in the Boltzmann equation and which gives the probability of finding  
 317 a particle at the position  $\mathbf{x}$ , at the time  $t$  and at the speed  $\mathbf{c}$ . Compared to  
 318 the Boltzmann equation, the velocity vector is discretized along directions in  
 319 the lattice Boltzmann equation, such as [46, 47]:

$$\frac{\partial f_i}{\partial t} + \mathbf{c}_i \cdot \nabla f_i = \Omega_i(\mathbf{f}) \quad \forall i \in \llbracket 0; I - 1 \rrbracket. \quad (13)$$

320 The notation  $\mathbf{f} = \{f_i\}_{i=0}^{I-1}$  will be used for the distribution function.  
 321 Such a notation will be used for other quantities, as soon as there is no  
 322 possible ambiguity. In two dimensions, the reference discretization scheme  
 323 involves  $I = 9$  discrete directions – yielding the so-called D2Q9 scheme. The  
 324 directions and associated weights are given by [48]:

$$\mathbf{c} = \begin{pmatrix} 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \end{pmatrix}, \quad (14)$$

325

$$\mathbf{w} = \left( \frac{4}{9} \quad \frac{1}{9} \quad \frac{1}{9} \quad \frac{1}{9} \quad \frac{1}{9} \quad \frac{1}{36} \quad \frac{1}{36} \quad \frac{1}{36} \quad \frac{1}{36} \right). \quad (15)$$

326 Also, from the definition of the velocity directions, it is convenient to  
 327 introduce the opposed velocity directions  $\bar{\mathbf{i}}$  with respect to  $\mathbf{c}_0$ , to write the  
 328 bounce-back boundary conditions:

$$\bar{\mathbf{i}} = (\bar{0} \quad \bar{1} \quad \bar{2} \quad \bar{3} \quad \bar{4} \quad \bar{5} \quad \bar{6} \quad \bar{7} \quad \bar{8}) = (0 \quad 3 \quad 4 \quad 1 \quad 2 \quad 7 \quad 8 \quad 5 \quad 6). \quad (16)$$

329 The lattice Boltzmann equation (13) is generally solved in two steps: the  
 330 collision step, and the streaming step. For the collision operator,  $\Omega(\mathbf{f})$ , the  
 331 simple model introduced by Bhatnagar-Gross-Krook (BGK) [49, 50] which  
 332 relies on a single-relaxation time (SRT) is often used. However, this is often  
 333 a source of spurious oscillations and instabilities as the Reynolds number  
 334 increases. As an example, d’Humières et al. [51] reported severe oscillations  
 335 for the pressure field in the cavity flow for the SRT model at  $\text{Re}=500$ . So,

336 in order to improve the numerical stability of the LBM, a multi-relaxation  
 337 time (MRT) operator has further been introduced [51]. It is written as:

$$\Omega(\mathbf{f}) = -\mathbf{M}^{-1}\mathbf{S}\mathbf{M}(\mathbf{f} - \mathbf{f}^{\text{eq}}), \quad (17)$$

338 in which  $\mathbf{M}$  is the transformation matrix between the moments and the  
 339 distribution functions:

$$\mathbf{M} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -4 & -1 & -1 & -1 & -1 & 2 & 2 & 2 & 2 \\ 4 & -2 & -2 & -2 & -2 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\ 0 & -2 & 0 & 2 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \\ 0 & 0 & -2 & 0 & 2 & 1 & 1 & -1 & -1 \\ 0 & 1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 \end{pmatrix}, \quad (18)$$

340 and  $\mathbf{S}$  is the diagonal relaxation rate matrix defined by [52]:

$$\mathbf{S} = \text{diag}(1, s_e, s_e, 1, s_q, 1, s_q, s_\nu, s_\nu). \quad (19)$$

341 Note that  $s_i = 1$  corresponds to conserved moments (conservation of mass  
 342 and momentum), and  $s_\nu$  is related to the fluid viscosity:

$$\frac{1}{s_\nu} = 3\nu + \frac{1}{2}. \quad (20)$$

343 The other components are to be adjusted in order to improve the nu-  
 344 merical stability and are often determined to be close to one through an  
 345 optimization process [53, 54]. In this article the fluid used in the cavity is  
 346 water, so an incompressible model is used for the LBM. The equilibrium  
 347 distribution  $f_i^{\text{eq}}$  is then given by [55, 56]:

$$f_i^{\text{eq}} = \omega_i \left( \rho + \rho_0 \left( 3\alpha(\mathbf{c}_i \cdot \mathbf{u}) + \frac{9}{2}\alpha(\mathbf{c}_i \cdot \mathbf{u})^2 - \frac{3}{2}\alpha\mathbf{u}^2 \right) \right). \quad (21)$$

348 The design-related variable  $\alpha(\psi(\mathbf{x}))$  involved in eq. (21) has been defined  
 349 in section 2. The macroscopic quantities, the fluid density  $\rho$ , the velocity  $\mathbf{u}$ ,  
 350 and the pressure can further be computed with the moments of  $\mathbf{f}$ :

$$\rho(\mathbf{x}, t) = \sum_{i=0}^8 f_i(\mathbf{x}, t), \quad \rho_0 \mathbf{u}(\mathbf{x}, t) = \sum_{i=0}^8 \mathbf{c}_i f_i(\mathbf{x}, t), \quad p(\mathbf{x}, t) = c_s^2 \rho(\mathbf{x}, t), \quad (22)$$

351 where  $\rho = \rho_0 + \delta\rho$ ,  $\delta\rho$  being the density fluctuation and **the mean density**  
 352  **$\rho_0$  is chosen to be equal to 1 in our simulations [56]**, and  $c_s = 1/\sqrt{3}$  the  
 353 lattice speed of sound. The fluid velocity needs to be very low compared  
 354 to  $c_s$  in order to satisfy the low mach number assumption required for the  
 355 equilibrium distribution function expansion [57]. **Compared to the classical**  
 356 **model, neglecting the density fluctuations in terms involving velocity induces**  
 357 **a decoupling between density and velocity [58]. While reducing the errors**  
 358 **due to compressibility [59], it should be noted that this model is only valid for**  
 359 **steady-state flows [60].** Next, the bounce-back boundary condition is applied  
 360 on all interfaces but on the inlet and outlet, where the boundary conditions  
 361 proposed by Zou and He [24] are applied. The user-parameter  $\epsilon$  involved  
 362 in (12) is chosen to tend to zero within this multi-relaxation time lattice  
 363 Boltzmann model, so that  $\alpha$  equals either 0 or 1, and a clear definition of the  
 364 topology is considered to avoid any bias in the fluid flow forward modeling.

### 365 3.2. Single-relaxation time model for the concentration distribution

366 Based on a double distribution function approach, a second distribution  
 367 function,  $\mathbf{g}$ , similar to  $\mathbf{f}$ , is introduced to solve the concentration field [34,  
 368 35]:

$$\frac{\partial g_i}{\partial t} + \mathbf{c}_i \cdot \nabla g_i + s_i = \Omega_i \quad \forall i \in \llbracket 0; I - 1 \rrbracket, \quad (23)$$

369 with the collision operator defined as:

$$\Omega_i = -\frac{1}{\tau_g} (g_i - g_i^{\text{eq}}). \quad (24)$$

370 Although the multi-relaxation time collision operator is used for the dis-  
 371 tribution function  $\mathbf{f}$ , the simpler single-relaxation time model is used here,  
 372 with only one relaxation time  $\tau_g$  for the distribution function  $\mathbf{g}$ . The lattice  
 373 Boltzmann equation for the concentration is more stable than the one for  
 374 the fluid flow, and the multi-relaxation time model is not mandatory for this  
 375 distribution function. Indeed, the SRT-BGK model is suitable to solve this  
 376 problem as long as the diffusion is isotropic [61, 62], which is the case here.  
 377 The relaxation time  $\tau_g$  is related to the mass diffusivity  $D$  of the chemical  
 378 species:

$$\tau_g = 3D + \frac{1}{2}. \quad (25)$$

379 In (23), the source term involved in the reaction process equation is dis-  
 380 tributed on all the discrete velocity directions, according to the D2Q9 scheme.

381 For a linear source term,  $s = k c_A$ , one can write:

$$s_i = \omega_i k c_A \quad \forall i \in \llbracket 0; I - 1 \rrbracket. \quad (26)$$

382 More generally, the LBM formulation for a given source model  $s$  is relaxed  
 383 towards the different velocities directions as follow:

$$s_i = \omega_i s. \quad (27)$$

384 The equilibrium distribution function  $g_i^{\text{eq}}$  is given by [63]:

$$g_i^{\text{eq}} = \omega_i c_A (1 + 3\alpha \mathbf{c}_i \cdot \mathbf{u}). \quad (28)$$

385 It can be noticed that the velocity field is used to compute this equilibrium  
 386 distribution function, illustrating the coupling between the concentration and  
 387 the velocity. The concentration  $c_A$  is computed with the zeroth order of the  
 388 distribution function  $\mathbf{g}$  such as [35] :

$$c_A(\mathbf{x}, t) = \sum_{i=0}^8 g_i(\mathbf{x}, t) \quad (29)$$

389 The mass flux is written as [14]:

$$\mathbf{q}(\mathbf{x}, t) = \sum_{i=0}^8 \mathbf{c}_i g_i(\mathbf{x}, t) - c_A \mathbf{u} \quad (30)$$

390 In order to implement the boundary conditions, the unknown distribu-  
 391 tion functions are assumed to be the equilibrium distribution functions with  
 392 the concentration  $c'_A$  to be determined [15, 64]. For the prescribed inlet con-  
 393 centration,  $c'_A$  is calculated by (29), with  $c_A = c_{A\text{in}}$ . At the outlet,  $c'_A$  is  
 394 calculated by (30), with  $\mathbf{q} = 0$ .

395

396 A similar solver has been validated for a fluid flow and heat transfer  
 397 problem by the authors [32]. In that case, the passive scalar approach is  
 398 also used, the only difference is that the concentration is replaced by the  
 399 temperature.

400 *3.3. Residual form*

401 In order to calculate the cost function gradient, the adjoint-state method  
 402 will be used, see section 4. In order to set it up, the forward problem,  
 403 which consists of both the multi-relaxation time model for the fluid-flow,  
 404 and the single-relaxation time model for the concentration distribution, is  
 405 written down in terms of residuals. We denote  $R$  and  $P$  the residuals for  
 406 the Boltzmann state equations, and the boundary conditions, respectively.  
 407 Further, we use the superscripts  $f$  and  $g$  for the fluid flow, and for the  
 408 concentration, respectively. Such residuals have to be written down for each  
 409 velocity direction. Added to that, the boundary  $\partial\mathcal{D}$  of the medium  $\mathcal{D}$   
 410 is partitioned with the inlet  $\mathcal{D}_{\text{in}}$ , the outlet  $\mathcal{D}_{\text{out}}$ , and the no-slip boundaries  
 411  $\mathcal{D}_{\text{ns}}$ . With such notations, the forward problem is concisely written as:

$$\begin{aligned}
 & \text{search } (f_i, g_i)(\mathbf{x}, t), \quad i \in \llbracket 0, \dots, 8 \rrbracket \text{ such that:} \\
 & \bullet \forall \mathbf{x} \in \mathcal{D} : \\
 & \quad R_i^f(\mathbf{f}, \alpha) = \frac{\partial f_i}{\partial t} + \mathbf{c}_i \cdot \nabla f_i + (\mathbf{M}^{-1} \mathbf{S} \mathbf{M} (\mathbf{f} - \mathbf{f}^{\text{eq}}))_i = 0, \\
 & \quad R_i^g(\mathbf{f}, \mathbf{g}, \alpha) = \frac{\partial g_i}{\partial t} + \mathbf{c}_i \cdot \nabla g_i + s_i + \frac{1}{\tau_g} (g_i - g_i^{\text{eq}}) = 0, \\
 & \bullet \forall \mathbf{x} \in \partial\mathcal{D}_{\text{in}} : \\
 & \quad P_1^f(\mathbf{f}) = f_1 - f_3 - \frac{2}{3}u_{\text{in}} = 0, \\
 & \quad P_5^f(\mathbf{f}) = f_5 - f_7 - \frac{1}{6}u_{\text{in}} - \frac{1}{2}(f_4 - f_2) = 0, \\
 & \quad P_8^f(\mathbf{f}) = f_8 - f_6 - \frac{1}{6}u_{\text{in}} + \frac{1}{2}(f_4 - f_2) = 0, \\
 & \quad P_1^g(\mathbf{g}) = g_1 - \frac{1}{9}\chi(1 + 3u_{\text{in}}) = 0, \\
 & \quad P_5^g(\mathbf{g}) = g_5 - \frac{1}{36}\chi(1 + 3u_{\text{in}}) = 0, \\
 & \quad P_8^g(\mathbf{g}) = g_8 - \frac{1}{36}\chi(1 + 3u_{\text{in}}) = 0, \\
 & \bullet \forall \mathbf{x} \in \partial\mathcal{D}_{\text{out}} : \\
 & \quad P_3^f(\mathbf{f}) = f_3 - f_1 + \frac{2}{3}\eta = 0, \\
 & \quad P_6^f(\mathbf{f}) = f_6 - f_8 + \frac{1}{6}\eta - \frac{1}{2}(f_4 - f_2) = 0, \\
 & \quad P_7^f(\mathbf{f}) = f_7 - f_5 + \frac{1}{6}\eta + \frac{1}{2}(f_4 - f_2) = 0, \\
 & \quad P_3^g(\mathbf{f}, \mathbf{g}) = g_3 - \frac{1}{9}\zeta(1 - 3\eta) = 0, \\
 & \quad P_6^g(\mathbf{f}, \mathbf{g}) = g_6 - \frac{1}{36}\zeta(1 - 3\eta) = 0, \\
 & \quad P_7^g(\mathbf{f}, \mathbf{g}) = g_7 - \frac{1}{36}\zeta(1 - 3\eta) = 0, \\
 & \bullet \forall \mathbf{x} \in \partial\mathcal{D}_{\text{ns}} : \\
 & \quad P_{(\mathbf{c}_i \cdot \mathbf{n} < 0)}^f(\mathbf{f}) = f_{(\mathbf{c}_i \cdot \mathbf{n} < 0)} - f_{(\mathbf{c}_i \cdot \mathbf{n} > 0)} = 0, \\
 & \quad P_{(\mathbf{c}_i \cdot \mathbf{n} < 0)}^g(\mathbf{g}) = g_{(\mathbf{c}_i \cdot \mathbf{n} < 0)} - g_{(\mathbf{c}_i \cdot \mathbf{n} > 0)} = 0,
 \end{aligned} \tag{31}$$



412 with:

$$\begin{aligned}
\eta &= -\rho_{\text{out}} + f_0 + f_2 + f_4 + 2(f_1 + f_5 + f_8), \\
\chi &= \frac{6(c_{A\text{in}} - g_0 - g_2 - g_3 - g_4 - g_6 - g_7)}{(1+3u_{\text{in}})}, \\
\zeta &= \frac{6(g_1 + g_5 + g_8)}{(1+3\eta)}.
\end{aligned} \tag{32}$$

### 413 3.4. LBM-based cost function

414 The cost function written in terms of the primal variables is given com-  
415 bining eqs. (7) and (8), which gives:

$$\mathcal{J}^+(\mathbf{u}, c_A, \Delta p) = \frac{1}{|\partial\mathcal{D}_{\text{out}}|} \int_{\partial\mathcal{D}_{\text{out}}} \mathbf{u} \cdot \mathbf{n} c_A \, d\mathbf{x} + \ell \Delta p_{\text{max}} \exp\left(\frac{\Delta p}{\Delta p_{\text{max}}}\right). \tag{33}$$

416 This cost function is to be re-written in terms of the lattice Boltzmann  
417 variables,  $\mathbf{f}$  and  $\mathbf{g}$ . Taking into account of the following relationships between  
418 the primal variables and the lattice Boltzmann variables:

$$\begin{aligned}
\mathbf{u} &= \sum_{i=0}^8 \mathbf{c}_i f_i(\mathbf{x}, t) \\
c_A &= \sum_{i=0}^8 g_i(\mathbf{x}, t) \\
\Delta p &= \frac{1}{|\partial\mathcal{D}_{\text{in}}|} \left[ \frac{1}{3} \int_{\partial\mathcal{D}_{\text{in}}} \sum_{i=0}^8 f_i \, d\mathbf{x} - \frac{1}{3} \int_{\partial\mathcal{D}_{\text{out}}} \sum_{i=0}^8 f_i \, d\mathbf{x} \right],
\end{aligned} \tag{34}$$

419 the cost function that is, finally, to be minimized is:

$$\begin{aligned}
\hat{\mathcal{J}}^+(\mathbf{f}, \mathbf{g}) &= \frac{1}{|\partial\mathcal{D}_{\text{out}}|} \int_{\partial\mathcal{D}_{\text{out}}} \sum_{i=0}^8 \mathbf{c}_i f_i \cdot \mathbf{n} \sum_{i=0}^8 g_i \, d\mathbf{x} \\
&+ \ell \Delta p_{\text{max}} \exp\left(\frac{\frac{1}{3} \int_{\partial\mathcal{D}_{\text{in}}} \sum_{i=0}^8 f_i \, d\mathbf{x}}{|\partial\mathcal{D}_{\text{in}}| \Delta p_{\text{max}}}\right).
\end{aligned} \tag{35}$$

420 Note that the pressure term at the outlet is not involved here. This one  
421 being considered as prescribed, the pressure difference is only driven by the  
422 modification of the inlet pressure during the optimization.

423 **4. The cost function gradient**

424 In order to derive the full adjoint-state problem needed for the com-  
 425 putation of the cost function gradient, the methodology and notations of  
 426 Gunzburger [65] are introduced:

- 427 •  $\mathbf{F}(\boldsymbol{\phi}, \Psi) = 0$  is the forward model gathering all the equations of eq. (31);
- 428 •  $\boldsymbol{\phi} = (\mathbf{f}, \mathbf{g})$  is the global forward state;
- 429 •  $\boldsymbol{\phi}^* = (\mathbf{f}^*, \mathbf{g}^*)$  is the global adjoint-state.

430 The Lagrange function associated to the optimization problem is written  
 431 as<sup>1</sup>:

$$\mathcal{L}(\boldsymbol{\phi}, \Psi, \boldsymbol{\phi}^*) = \widehat{\mathcal{J}}^+(\boldsymbol{\phi}) + \langle \mathbf{F}(\boldsymbol{\phi}, \Psi), \boldsymbol{\phi}^* \rangle. \quad (37)$$

432 The optimization problem is solved searching for the stationary point of  
 433 the Lagrange function. This point satisfies:

$$\delta\mathcal{L} = \frac{\partial\mathcal{L}}{\partial\boldsymbol{\phi}}\delta\boldsymbol{\phi} + \frac{\partial\mathcal{L}}{\partial\Psi}\delta\Psi + \frac{\partial\mathcal{L}}{\partial\boldsymbol{\phi}^*}\delta\boldsymbol{\phi}^* = 0, \quad (38)$$

434 where  $\delta\mathcal{L}$ ,  $\delta\boldsymbol{\phi}$ ,  $\delta\Psi$  and  $\delta\boldsymbol{\phi}^*$  stand for arbitrary variations [65]. Three terms  
 435 appear in the right hand side of (38):

- 436 • the first term, the differential with respect to the state,  $\partial\mathcal{L}/\partial\boldsymbol{\phi}$ , yields  
 437 the adjoint-state equation;
- 438 • the second term, the differential with respect to the design variables,  
 439  $\partial\mathcal{L}/\partial\Psi$ , yields the optimality conditions;

---

<sup>1</sup>With the notations given above, this eq. (37) can be straitforwardly expanded to:

$$\begin{aligned} \mathcal{L}(\mathbf{f}, \mathbf{g}, \Psi, \mathbf{f}^*, \mathbf{g}^*) = & \widehat{\mathcal{J}}^+(\mathbf{f}, \mathbf{g}) + \int_0^{t_f} \left( \int_{\mathcal{D}} \sum_{\substack{q=\{f,g\} \\ i=0,\dots,8}} R_i^q q_i^* \, d\mathbf{x} \right. \\ & \left. + \left( \int_{\partial\mathcal{D}_{\text{in}}} \sum_{\substack{q=\{f,g\} \\ i=\{1,5,8\}}} + \int_{\partial\mathcal{D}_{\text{out}}} \sum_{\substack{q=\{f,g\} \\ i=\{3,6,7\}}} + \int_{\partial\mathcal{D}_{\text{ns}}} \sum_{\substack{q=\{f,g\} \\ \mathbf{c}_i \cdot \mathbf{n} < 0}} \right) (P_i^q q_i^* \, d\mathbf{x}) \right) dt. \end{aligned} \quad (36)$$

440 • the third term, the differential with respect to the adjoint-state vari-  
441 able,  $\partial\mathcal{L}/\partial\phi^*$ , yields back the equations of the forward model that are  
442 to be satisfied.

443 A similar derivation of the adjoint-state problem for a convective fluid  
444 flow problem has been detailed by the authors [15]. Based on this method,  
445 the adjoint-state is finally written as :

search  $(f_i^*, g_i^*)(\mathbf{x}, t)$ ,  $i \in \llbracket 0, \dots, 8 \rrbracket$ , with  $(f_i, g_i)(\mathbf{x}, t)$  given by (31), such that:

•  $\forall \mathbf{x} \in \mathcal{D}$  :

$$\begin{aligned} R_i^{*,f}(\mathbf{f}, \mathbf{g}, \mathbf{f}^*, \mathbf{g}^*, \alpha) &= -\frac{\partial f_i^*}{\partial t} - \mathbf{c}_i \cdot \nabla f_i^* + (\mathbf{M}^{-1} \mathbf{S} \mathbf{M} (\mathbf{f}^* - \mathbf{f}^{*,\text{eq}}))_i + Q_i^{*,f} = 0, \\ R_i^{*,g}(\mathbf{f}, \mathbf{g}, \mathbf{g}^*, \alpha) &= -\frac{\partial g_i^*}{\partial t} - \mathbf{c}_i \cdot \nabla g_i^* + \frac{1}{\tau_g} (g_i^* - g_i^{*,\text{eq}}) + Q_i^{*,g} = 0, \end{aligned}$$

•  $\forall \mathbf{x} \in \partial \mathcal{D}_{\text{in}}$  :

$$\begin{aligned} P_3^{*,f}(\mathbf{f}^*, \mathbf{f}) &= f_3^* - f_1^* + \ell \frac{1}{3|\partial \mathcal{D}_{\text{in}}|} \exp \left( \frac{\frac{1}{3} \int_{\partial \mathcal{D}_{\text{in}}} \sum_{i=0}^8 f_i \, d\mathbf{x}}{|\partial \mathcal{D}_{\text{in}}| \Delta p_{\text{max}}} \right) \\ P_7^{*,f}(\mathbf{f}^*, \mathbf{f}) &= f_7^* - f_5^* + \ell \frac{1}{3|\partial \mathcal{D}_{\text{in}}|} \exp \left( \frac{\frac{1}{3} \int_{\partial \mathcal{D}_{\text{in}}} \sum_{i=0}^8 f_i \, d\mathbf{x}}{|\partial \mathcal{D}_{\text{in}}| \Delta p_{\text{max}}} \right) \\ P_6^{*,f}(\mathbf{f}^*, \mathbf{f}) &= f_6^* - f_8^* + \ell \frac{1}{3|\partial \mathcal{D}_{\text{in}}|} \exp \left( \frac{\frac{1}{3} \int_{\partial \mathcal{D}_{\text{in}}} \sum_{i=0}^8 f_i \, d\mathbf{x}}{|\partial \mathcal{D}_{\text{in}}| \Delta p_{\text{max}}} \right) \\ P_3^{*,g}(\mathbf{g}^*) &= g_3^* + \frac{1}{6} (4g_1^* + g_5^* + g_8^*) \\ P_6^{*,g}(\mathbf{g}^*) &= g_6^* + \frac{1}{6} (4g_1^* + g_5^* + g_8^*) \\ P_7^{*,g}(\mathbf{g}^*) &= g_7^* + \frac{1}{6} (4g_1^* + g_5^* + g_8^*) \end{aligned}$$

•  $\forall \mathbf{x} \in \partial \mathcal{D}_{\text{out}}$  :

$$\begin{aligned} P_1^{*,f}(\mathbf{f}^*, \mathbf{g}^*, \mathbf{f}, \mathbf{g}) &= f_1^* - f_3^* + \frac{1}{3} (4f_3^* + f_6^* + f_7^*) + \frac{1}{6} \left( \frac{\zeta}{1+3\eta} \right) (4g_3^* + g_6^* + g_7^*) + \frac{c_A(\mathbf{g})}{|\partial \mathcal{D}_{\text{out}}|} = 0 \\ P_5^{*,f}(\mathbf{f}^*, \mathbf{g}^*, \mathbf{f}, \mathbf{g}) &= f_5^* - f_7^* + \frac{1}{3} (4f_3^* + f_6^* + f_7^*) + \frac{1}{6} \left( \frac{\zeta}{1+3\eta} \right) (4g_3^* + g_6^* + g_7^*) + \frac{c_A(\mathbf{g})}{|\partial \mathcal{D}_{\text{out}}|} = 0 \\ P_8^{*,f}(\mathbf{f}^*, \mathbf{g}^*, \mathbf{f}, \mathbf{g}) &= f_8^* - f_6^* + \frac{1}{3} (4f_3^* + f_6^* + f_7^*) + \frac{1}{6} \left( \frac{\zeta}{1+3\eta} \right) (4g_3^* + g_6^* + g_7^*) + \frac{c_A(\mathbf{g})}{|\partial \mathcal{D}_{\text{out}}|} = 0 \\ P_1^{*,g}(\mathbf{g}^*, \mathbf{f}) &= g_1^* - \frac{1}{6} \left( \frac{1-3\eta}{1+3\eta} \right) (4g_3^* + g_6^* + g_7^*) + \frac{\eta}{|\partial \mathcal{D}_{\text{out}}|} \\ P_5^{*,g}(\mathbf{g}^*, \mathbf{f}) &= g_5^* - \frac{1}{6} \left( \frac{1-3\eta}{1+3\eta} \right) (4g_3^* + g_6^* + g_7^*) + \frac{\eta}{|\partial \mathcal{D}_{\text{out}}|} \\ P_8^{*,g}(\mathbf{g}^*, \mathbf{f}) &= g_8^* - \frac{1}{6} \left( \frac{1-3\eta}{1+3\eta} \right) (4g_3^* + g_6^* + g_7^*) + \frac{\eta}{|\partial \mathcal{D}_{\text{out}}|} \end{aligned}$$

•  $\forall \mathbf{x} \in \partial \mathcal{D}_{\text{ns}}$  :

$$\begin{aligned} P_{(\mathbf{c}_i \cdot \mathbf{n} > 0)}^{*,f}(\mathbf{f}^*) &= f_{(\mathbf{c}_i \cdot \mathbf{n} > 0)}^* - f_{(\mathbf{c}_i \cdot \mathbf{n} < 0)}^* = 0, \\ P_{(\mathbf{c}_i \cdot \mathbf{n} > 0)}^{*,g}(\mathbf{g}^*) &= g_{(\mathbf{c}_i \cdot \mathbf{n} > 0)}^* - g_{(\mathbf{c}_i \cdot \mathbf{n} < 0)}^* = 0. \end{aligned}$$

(39)

446 with:

$$\begin{aligned}
f_i^{*,\text{eq}} &= \sum_{j=0}^8 \frac{\partial f_j^{\text{eq}}}{\partial f_i} f_j^*, \\
Q_i^{*,f} &= \sum_{j=0}^8 -g_j^* \left( \frac{3\omega_j c_A}{\tau_g} \right) \mathbf{c}_j \cdot \mathbf{c}_i, \\
g_i^{\text{eq},*} &= \sum_{j=0}^8 \frac{\partial g_j^{\text{eq}}}{\partial g_i} g_j^*, \\
Q_i^{*,g} &= \sum_{j=0}^8 \frac{\partial s_j}{\partial g_i} g_j^*, \\
\eta &= -\rho_{\text{out}} + f_0 + f_2 + f_4 + 2(f_1 + f_5 + f_8), \\
\zeta &= \frac{6(g_1 + g_5 + g_8)}{(1+3\eta)}.
\end{aligned} \tag{40}$$

To compute the different adjoint-state variables, the steady-state solution of the forward problem is used. The adjoint-states being computed, the cost function gradient is finally computed through

$$\begin{aligned}
\nabla_{\Psi} \widehat{\mathcal{J}}^+ (\mathbf{f}, \mathbf{g}, \mathbf{f}^*, \mathbf{g}^*) &= \\
& - \alpha'(\Psi) \int_0^{t_f} \sum_{i=0}^8 \omega_i f_i^* \left( \mathbf{M}^{-1} \mathbf{S} \mathbf{M} \left( 3 \mathbf{c}_j \cdot \mathbf{u} + \frac{9}{2} (\mathbf{c}_j \cdot \mathbf{u})^2 - \frac{3}{2} \mathbf{u}^2 \right) \right)_i dt \\
& - \alpha'(\Psi) \int_0^{t_f} \sum_{i=0}^8 \frac{3 \omega_i g_i^* c_A \mathbf{c}_i \cdot \mathbf{u}}{\tau_g} dt. \tag{41}
\end{aligned}$$

447 The general topology optimization algorithm is detailed in Algorithm 1.  
448 The iterative algorithm involves a criterion based on the stabilization of the  
449 cost function value which is detailed in the next section.

---

**Algorithm 1:** General topology optimization algorithm

---

**Input:** Level-set function  $\Psi^{(0)}$ ;

Topology  $\mathcal{T}^{(0)}$  through  $\alpha^{(0)}$  (see eq. (10)), along with the smooth version eq. (12) ;

**while** *criterion* (43) *not satisfied* **do**

    Compute the Boltzmann variables  $\mathbf{f}$  and  $\mathbf{g}$  solving eq. (31);

    Compute the cost function value  $\widehat{\mathcal{J}}^+(\mathbf{f}, \mathbf{g})$  with eq. (35);

    Compute the adjoint Boltzmann variables  $\mathbf{f}^*$  and  $\mathbf{g}^*$  solving eq. (39);

    Compute the cost function gradient  $\nabla_{\Psi} \widehat{\mathcal{J}}^+$  from eq. (41);

    Update of the geometry : actualization of the level-set function with eq. (9);

**return** *Optimal topology*  $\mathcal{T}^{(*)}$ ;

---

450 **5. Test cases and results**

451 For the validation of the proposed method, the reader is referred to a  
 452 previous work of the authors [15] where a thermal fluid flow topology op-  
 453 timization case has been computed by following a similar procedure. The  
 454 obtained results have been then compared with a benchmark test in liter-  
 455 ature and a study about the grid independency and the sensitivity of the  
 456 algorithm to different initializations have also been conducted.

457  
 458 The geometry and the configuration of the test cases are shown on fig. 1.  
 459 The 2D square domain is enclosed by no-slip walls. The gray layers, shown  
 460 on fig. 1, represent the fixed solid boundary, on which the no-slip condition  
 461 is applied. The cavity contains the fluid-solid distribution, and the set of  
 462 inlet/outlet is also schematically represented. At the inlet,  $\partial\mathcal{D}_{\text{in}}$ , the fluid  
 463 enters with a parabolic velocity profile.

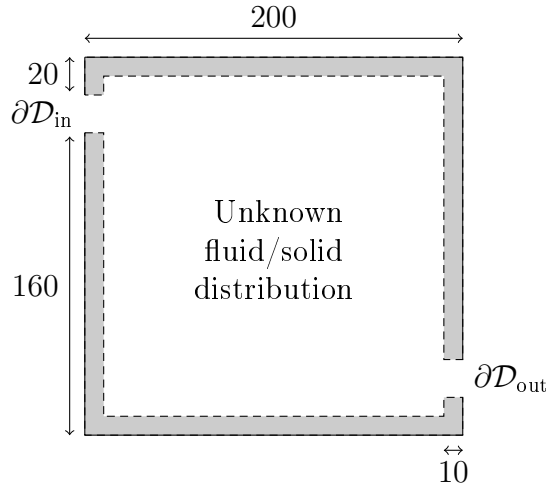


Figure 1: Schematic representation of the optimization problem configuration.

464 The convergence criterion for both the forward LBM problem and the  
 465 adjoint-state LBM problem has been chosen to be:

$$\frac{\|a^{(n)} - a^{(n-10,000)}\|_{\infty}}{\|a^{(n-10,000)}\|_{\infty}} < 10^{-4} \quad \text{with} \quad \|a^{(n)}\|_{\infty} = \max_{\substack{q=\{f,g\} \\ j=0,\dots,8 \\ i=1,\dots,N}} |q_j^{(n)}(x_i)|, \quad (42)$$

466 in which the infinity norm is applied on the vector involving all the nine  
 467 directions, and all spatial nodes, for both quantities, and the superscript ( $n$ )  
 468 stands for the LBM iteration count. Besides, the convergence criterion of the  
 469 optimization problem is based on the stabilization of the cost function value  
 470 along with ten successive iterations:

$$\left| \frac{\mathcal{J}^{(k)} - \mathcal{J}^{(k-10)}}{\mathcal{J}^{(k-10)}} \right| < 10^{-4}, \quad (43)$$

471 where  $\mathcal{J}^{(k)}$  is the cost function value at the iteration count  $k$ . Calculations  
 472 were performed on a NVIDIA Quadro K6000 GPU card for taking advantage  
 473 of the LBM algorithm parallelism. Normally, for the adjoint-states calcula-  
 474 tion, one needs to store the macroscopic values of the forward problem, at  
 475 each LBM iteration, which is prohibitive in terms of memory requirement.  
 476 Only steady-state problems are considered here, so, as stated by [29], the  
 477 solution of the forward problem at final time can be used as the stationary  
 478 source term for the whole adjoint-states calculation.

479 Regarding the reaction source term, instead of the simple linear model  
 480 introduced previously in the adimensionnalised Damkohler number, a two-  
 481 parameters model is chosen for a more tunable reaction:

$$s = k(1 - \exp(-rc_A)), \quad (44)$$

482 The coefficient  $k$  controls the maximum reaction rate, and  $r$  is a positive  
 483 user-defined parameter that controls the dependency to the concentration: a  
 484 high value prescribes a quasi-independent concentration rate whereas a small  
 485 value tends to a linear model.

486 The numerical examples presented in this section use the following pa-  
 487 rameters:

- 488 • the spatial discretization for the domain is  $200 \times 200$  elements,
- 489 • the reaction rate coefficient  $k$  is equal to  $2 \times 10^{-5}$ ,
- 490 • the Peclet number  $Pe$  is 2000,
- 491 • the initialization starts with the full fluid topology, i.e. with  $\Psi(\mathbf{x}) > 0$ ,
- 492 • the iteration matrix  $\mathbf{P}$  used for the level-set function evolution in eq. (9)  
 493 is chosen to be a diagonal matrix satisfying  $\mathbf{P}_i = 0.01/\alpha'(\Psi_i)$ . The benefit



494 of this choice is threefold: i) the derivative  $\alpha'(\Psi) \geq 0$  is no longer in-  
495 volved in the level-set function evolution, so even a discontinuous func-  
496 tion  $\alpha(\Psi)$  can be used; ii) the user-parameter  $\epsilon$  is not to be pre-assigned  
497 to a given value, this parameter being no longer involved anywhere in  
498 the optimization process; iii) there is no more bias between the response  
499 of the forward model, i.e. the value of the cost function  $\mathcal{J}$  which would  
500 need  $\epsilon = 0$ , and its gradient,  $\nabla_{\Psi}\mathcal{J}$ , which would need  $\epsilon \neq 0$  for its  
501 existence condition. Next, the descent parameter 0.01 involved at the  
502 numerator of the iteration matrix, has been chosen following Dugast et  
503 al. [15].

- 504 • the maximal allowed pressure drop is twice the initial pressure drop  
505 (calculated at the first iteration with the full fluid geometry),
- 506 • the relaxation times for the MRT are set to  $s_e = s_\epsilon = s_q = 0.6$  and  
507  $s_\nu = 1/(3\nu + 0.5)$ .
- 508 • the reaction rate coefficient  $r$  is equal to 10, which corresponds to a  
509 Damkholer number  $Da$  equal to 0.1.

510 As the MRT model allows the calculation of higher Reynolds number  
511 flows compared to the SRT model, the first study described hereafter is based  
512 on the influence of the Reynolds number on the optimized topology. Three  
513 cases are presented :  $Re = 10$ ,  $Re = 100$  and  $Re = 1000$ . It is to be noticed  
514 that although the forward and adjoint-state problems could have been solved  
515 with the single-relaxation time model, for both  $Re = 10$  and  $Re = 100$ , the  
516 convergence of the LBM solver is not possible without a modification of the  
517 relaxation times  $s_{0-6}$  for  $Re = 1000$ . This study shows that the introduction  
518 of the solid parts breaks the main fluid flow path going from the inlet to  
519 the outlet via the center of the domain into several fluid paths. This is true  
520 for the three tested Reynolds numbers. This path division participates to a  
521 better distribution of the fluid flow on the entire domain, especially on the  
522 top-right and bottom-left corners compared to the initial configuration. One  
523 can notice that the complexity of the flow paths increases with the Reynolds  
524 number. Apart from advection, the forward problem involves also diffusion  
525 and reaction phenomena. Consequently, the second study deals with the  
526 influence of the mass diffusivity and of the reaction rate on the obtained  
527 topology. The modification of the mass diffusivity affects the balance between  
528 advection and diffusion and therefore the impact of the fluid flow velocity on

529 the concentration. The reaction rate is used to control the speed on the  
 530 reaction. The influence of a faster reaction will be studied. With these two  
 531 studies, the topology optimization method has been tested for different flow  
 532 regimes and reactants. It shows its ability to produce specific optimized  
 533 topologies for a variety of configurations.

### 534 5.1. Influence of the Reynolds number

535 The first study deals with the influence of the Reynolds number on the  
 536 obtained optimized topology. The objective is the maximization of the re-  
 537 action within the domain, this measurement being calculated at the out-  
 538 let, see eq. (35). For this study, the Peclet number is kept constant. As  
 539  $Pe = Re \times Sc$ , it means that the Schmidt number is also modified along with  
 540 the Reynolds number.

#### 541 5.1.1. Case 1 : $Re = 10$

542 Figure 2 presents the results of the optimization process along with the  
 543 iterations, for the first case, with  $Re = 10$ . On the top and left-hand side is  
 544 presented the evolution of both the cost function value (mean of  $u \times c_{out}$ ),  
 545 and of the pressure drop ratio  $\frac{\Delta p}{\Delta p_{max}}$ , along with the iteration count. On the  
 546 right-hand side, is presented the evolution of the topology:  $\mathcal{T}_{[Re=10]}^{(0)}$  at the  
 547 iteration 0 (it is the initial guess),  $\mathcal{T}_{[Re=10]}^{(30)}$  at the iteration 30,  $\mathcal{T}_{[Re=10]}^{(50)}$  at the  
 548 iteration 50, and after reaching the stabilization of the cost function value,  
 549  $\mathcal{T}_{[Re=10]}^*$ , at the iteration 900.

550 From this figure it is seen that the solid parts are introduced only in the  
 551 center of the domain, but not close to both the inlet and the outlet. That is  
 552 the reason why the increase in the pressure drop ratio is not much, and the  
 553 constraint on the pressure drop is by far fulfilled. In fact, the introduction of  
 554 the solid medium close to the center of the medium divides the flow in two  
 555 distinct paths, as can be seen from fig. 2, in the middle. This makes such  
 556 that the fluid velocity is greater elsewhere, especially close to the bottom  
 557 right and top left corners. The effect is that more reactant is consumed in  
 558 these areas; this participates to the high decrease of the outlet concentration  
 559 (see the bottom of fig. 2). Note that, from the initial guess to the optimized  
 560 topology, the cost function has decreased from  $5.10^{-3}$  (LB unit) down to  
 561  $1.96.10^{-3}$  (LB unit), i.e. by a factor more than 2.5.

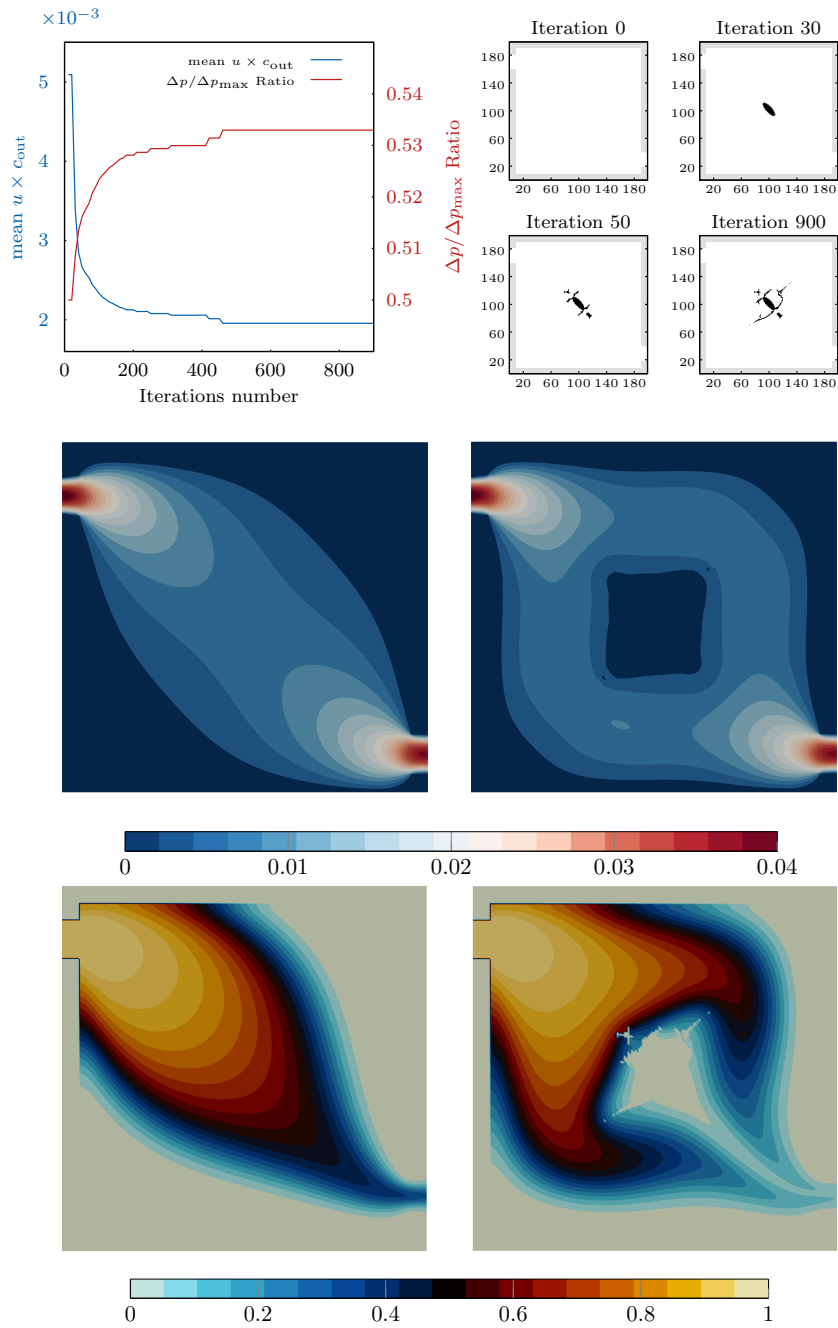


Figure 2:  $Re=10$ . Top left: evolution of the cost function and of the pressure drop ratio along with the iteration count. Top right: the topology at iterations 0, 30, 50, and 900.

Middle: module of the velocity field. Left: guess configuration (full fluid). Right: optimized topology. Bottom: concentration field. Left: guess configuration (full fluid). Right: optimized topology.

562 *5.1.2. Case 2 : Re =100*

563 Figure 3 presents the results of the optimization process along with the  
564 iterations, for the second case, with  $Re = 100$ . On the top and left-hand side  
565 is presented the evolution of both the cost function value (mean of  $u \times c_{out}$ ),  
566 and of the pressure drop ratio  $\frac{\Delta p}{\Delta p_{max}}$ , along with the iteration count. On the  
567 right-hand side, is presented the evolution of the topology:  $\mathcal{T}_{[Re=100]}^{(0)}$  at the  
568 iteration 0 (it is the initial guess),  $\mathcal{T}_{[Re=100]}^{(20)}$  at the iteration 20,  $\mathcal{T}_{[Re=100]}^{(50)}$  at the  
569 iteration 50, and after reaching the stabilization of the cost function value,  
570  $\mathcal{T}_{[Re=100]}^*$ , at the iteration 390. Comparing fig. 3 with fig. 2, it can be seen  
571 that the decrease of the cost function is more important for  $Re=100$  than for  
572  $Re=10$ . Here, the cost function has decreased from  $6.1 \cdot 10^{-3}$  (LB unit) down  
573 to  $5.96 \cdot 10^{-4}$  (LB unit), i.e. by a factor greater than 10 .

574 Conversely to the previous case with  $Re=10$ , the optimal fluid/solid con-  
575 figuration is here composed of several parts, located near the diagonal of the  
576 domain, facing the main fluid flow stream. The fluid flow is thus mainly  
577 directed towards the corners, but also a part of it goes through the center  
578 of the domain, as the solid line is not continuous, containing some holes, see  
579 the plot in the middle of fig. 3.

580 The outlet concentration for the optimized geometry is very close to zero,  
581 as can be seen from the plot in the bottom of fig. 3. This means that almost  
582 all the reactant has been consumed inside the domain. In that sense, the  
583 efficiency of the chemical reaction has been highly increased.

584 *5.1.3. Case 3 : Re =1000*

585 In this last test case about the Reynolds number study, the velocity and  
586 concentration fields for  $Re = 1000$  are radically different to previous cases,  
587 with  $Re = 10$  and  $Re = 100$ . As a matter of fact, the fig. 4 is to be compared  
588 to fig. 2 and fig. 3, middle and left-hand side for the velocity, and bottom and  
589 left-hand side for the concentration, at the initial guess, i.e. for the full fluid  
590 flow case. In fact, when  $Re = 1000$ , a re-circulation zone appears around  
591 the center of the domain. As a consequence, the concentration is very small  
592 there at the center of the vortex, but the concentration remains very high at  
593 the outlet.

594 The fluid/solid configuration found by the implemented topology opti-  
595 mization algorithm is, indeed, very far away from an optimized one, as the  
596 optimization process is struggling to find any proper topology. In order to  
597 facilitate the convergence of the optimization problem, the initial configura-

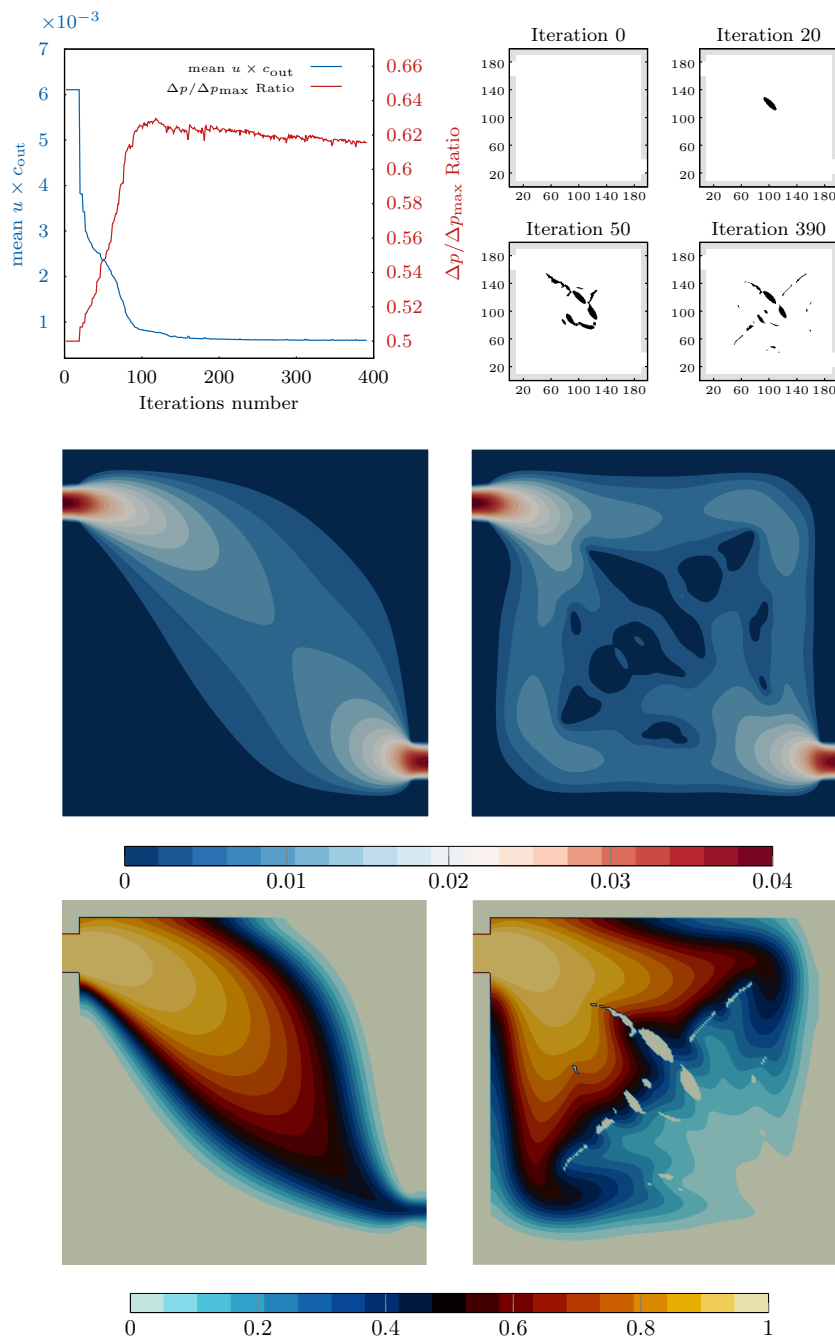


Figure 3:  $Re=100$ . Top left: evolution of the cost function and of the pressure drop ratio along with the iteration count. Top right: the topology at iterations 0, 20, 50, and 390.

Middle: module of the velocity field. Left: guess configuration (full fluid). Right: optimized topology.

Bottom: concentration field. Left: guess configuration (full fluid). Right: optimized topology.

598 tion was set to a uniform distribution of small solid circles inside the domain.  
599 With such an initialization, the re-circulation disappears, and the research of  
600 optimized geometries is easier. Note that the cost function value for the full  
601 fluid geometry was  $12.6 \cdot 10^{-3}$  (LB unit) while it is now  $4.5 \cdot 10^{-3}$  (LB unit)  
602 with this initialization, i.e. with circles.

603 The evolution along with the optimization iterations of the cost function  
604 and of the pressure drop limitation are shown on fig. 5, for this case. At  
605 the beginning of the optimization process, the pressure drop increases. This  
606 is due to the fact that some solid parts are introduced at the outlet of the  
607 domain. This may be seen as a drawback, but in fact, this also participates  
608 to the decrease of the concentration field at the outlet, which is the main  
609 objective of the optimization problem. Then, after some iterations, the limi-  
610 tation of the pressure drop included in the augmented cost function helps to  
611 prevent from the introduction of more solid parts near this area. The differ-  
612 ent solid parts introduced inside the domain are found to be very small: it is  
613 even difficult to see the difference between the different optimization steps,  
614 without a close look. But these small modifications have a huge impact on  
615 the cost function decrease.

616 As can be seen on fig. 5, a fluid path has been drawn on the left-hand side  
617 of the domain, by removing some solid elements from the initial topology.  
618 The distribution of the reactant is then more uniform, and the reaction rate is  
619 more important in this area, which participates to a diminution of the outlet  
620 concentration, as can be seen on the plot on the bottom of fig. 5. In that  
621 case again, the efficiency of the chemical reaction has been highly increased.

#### 622 *5.1.4. Crosscheck of the different optimized configurations*

623 Based on the Reynolds number test cases, a crosscheck comparison of  
624 the different optimal topologies has been performed in order to discuss on  
625 the results. In this additional study, the fluid flow with Reynolds numbers  
626 equal to 10, 100, and 1000 is applied on the three previously obtained opti-  
627 mal topologies. The cost function measuring the reaction efficiency is then  
628 calculated for each of these nine cases. The results are reported in table 1.  
629 The first row is related to the three different found optimal topologies, and  
630 the first column is related to the Reynolds number which is applied. The  
631 other numbers are the values of the calculated cost function.

632 The expected result is that the minimum value of the cost function is  
633 to be found for the applied Reynolds number equal to the one related to  
634 its optimal geometry. For readability considerations, the minimum value of

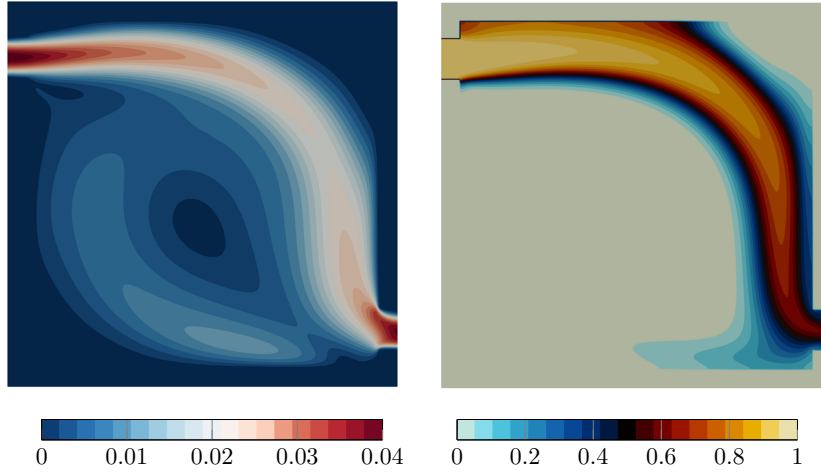


Figure 4: Re=1000. Velocity (left) and concentration (right) fields for the full fluid topology.

	$\mathcal{T}_{[\text{Re}=10]}^*$	$\mathcal{T}_{[\text{Re}=100]}^*$	$\mathcal{T}_{[\text{Re}=1000]}^*$
Re =10	1.9	<b>0.8</b>	2.6
Re =100	2.3	<b>0.59</b>	2.6
Re =1000	12.6	8.4	<b>0.49</b>

Table 1: Cost function values ( $\times 10^{-3}$ ) for different configurations

635 the cost function for each Reynolds number is written in bold characters,  
 636 in table 1.

637 For the applied Reynolds number equal to 100, one can see that the  
 638 related optimized topology,  $\mathcal{T}_{[\text{Re}=100]}^*$ , provides, by far, the best result. The  
 639 same trend is observed for the applied Reynolds number equal to 1000, but  
 640 with even a higher difference between the three topologies: the cost function  
 641 is equal to 0.49 with the topology  $\mathcal{T}_{[\text{Re}=1000]}^*$ , while it is equal to 8.4 and 12.6,  
 642 for topologies  $\mathcal{T}_{[\text{Re}=100]}^*$  and  $\mathcal{T}_{[\text{Re}=10]}^*$ , respectively.

643 However, for the applied Reynolds number equal to 10, it is seen from ta-  
 644 ble 1 that the minimum cost function value is given for the topology  $\mathcal{T}_{[\text{Re}=100]}^*$ .  
 645 This highlights that the topology obtained at the end of the optimization pro-  
 646 cess, after convergence, for the case of Re = 10, is a local minimum. Even  
 647 if this crosscheck did not show a local minimum for the two other configura-  
 648 tions, it is to be noticed that this does not mean that the global minimum

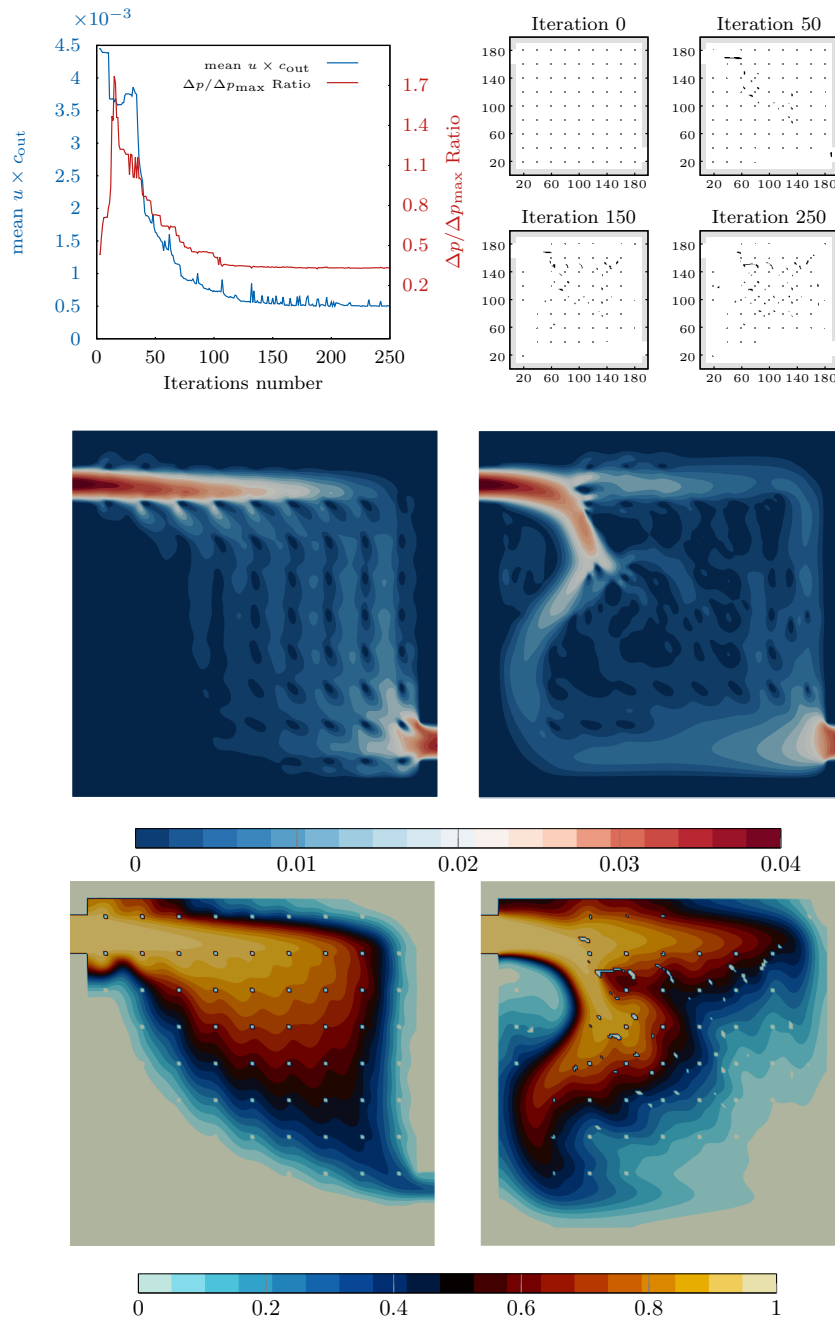


Figure 5:  $Re=1000$ . Top left: evolution of the cost function and of the pressure drop ratio along with the iteration count. Top right: the topology at iterations 0, 50, 150, and 250. Middle: module of the velocity field. Left: guess configuration. Right: optimized topology. Bottom: concentration field. Left: guess configuration. Right: optimized topology.



649 has been actually reached. In fact, it is well known that gradient-type meth-  
650 ods, because they are based on a local study of the function to be minimized,  
651 usually reach a local minimum next to the initial guess [66]. This is usually  
652 considered as the main drawback of these gradient-type algorithms. But,  
653 at the same time, compared to gradient-free optimization methods – which,  
654 indeed, are more likely to find the global minimum, gradient-type algorithms  
655 reach the minima much more efficiently. This point makes the difference.  
656 In fact, the optimization problem treated here involves  $200 \times 200$  unknowns;  
657 such a discretization would be impracticable with any gradient-free optimizer.  
658 This difficulty could of course be overcome by modifying the initial topology,  
659 many times, but, as the physical problem is complex, it will remain difficult  
660 (and likely impossible) to find the unique global minimum.

661 In further perspectives, the local minimum treatment is an interesting  
662 issue to solve, despite the fact that it can be difficult to avoid them while  
663 using a gradient-based optimization method. Nevertheless, one possibility  
664 would be to use a multi-scale resolution approach. Such a multi-resolution  
665 approach, formalized by Liu [67] for solving some ill-posed inverse problems,  
666 has been later on successfully used by Dubot et al. [68] and Liu [69], for  
667 example. In the framework of reactive fluid flow topology optimization, the  
668 use of a multi-scale resolution approach would enable to perform a scale-by-  
669 scale optimization on successive convex cost functions, following the work  
670 of Chavent [70]. Moreover, added to this interesting property, this would  
671 also save computational time due to faster convergence. This point will be  
672 addressed in a future research.

673 Following the study of the Reynolds number, the influence of both the  
674 reaction rate and diffusion is investigated. Additionally, the Damkohler and  
675 Peclet number are modified to determine their effect on the resultant system  
676 geometry.

### 677 5.2. Case 4 : Influence of the Damkohler number

678 The reaction rate  $k$  is now modified in order to evaluate the influence of  
679 the Damkohler number on the optimal topology. It has been increased from  
680  $2 \times 10^{-5}$  to  $4 \times 10^{-5}$ . Though this modification does not have any impact on  
681 the velocity, the concentration field is altered, as the reactant is consumed  
682 faster. This effect is clearly visible by comparing figs. 5 and 6.

683 Concerning the optimization results, one can observe a similar trend be-  
684 tween this case and the previous case 3. First, the evolution of the cost  
685 function and the pressure drop ratio, represented on the top of fig. 6, are

686 similar: one observes an increase and then a decrease of the pressure drop  
687 ratio, while the outlet concentration is decreasing. The optimal topology is  
688 also comparable to the one of case 3: it implies the same modification on  
689 the velocity in which the flow is divided into two main streams just after the  
690 inlet. The main difference between both the previous case 3 and this case 4  
691 is in the magnitude of the outlet concentration. This one is much smaller for  
692 the higher Damkholer number, as it was expected.

693 One can also see from fig. 7 (left) that the solid part at the core of the  
694 domain is denser for  $Da=0.1$  (in red) than for  $Da=0.2$  (in blue). Please note  
695 that, to enhance readability, the solid parts have been represented larger (in  
696 this figure only). For  $Da=0.2$ , because the reactant is consumed faster (with  
697 respect to  $Da=0.1$ ), it is consequently easier to obtain a small concentration  
698 at the outlet, even without the need to alter the velocity field through the  
699 addition of significant solid material. The comparison of the concentration  
700 field for the two Damkholer numbers is shown on fig. 7 (right). The threshold  
701  $c_A \geq 0.05$  is applied to the concentration field to get a better contrast between  
702 the two cases. For the higher Damkholer number, one can see that the  
703 concentration becomes very low shortly after the middle of the domain. As  
704 the reactant has been almost entirely consumed, the efficiency has been highly  
705 increased regarding to the cost function. However, the other conclusion that  
706 can be made based on this result is that the reactor has been over-sized for  
707 this reaction rate. In fact, based on the concentration field obtained for the  
708 optimized geometry, one can conclude that a good efficiency could have also  
709 been achieved with a smaller reactor. The real cost of the chemical reactor  
710 and the dimensions associated with it were not included in the optimization  
711 problem; it is nevertheless a useful conclusion from an engineering point of  
712 view.

### 713 5.3. Case 5 : Influence of the Peclet number

714 In the previous numerical examples, the Peclet number was equal to 2000.  
715 The advection process played a major role compared to the diffusion process.  
716 In this test case 5, the Peclet number is modified to be equal to 100. For the  
717 rest, the configuration is kept the same as for the previous case 3, and the  
718 Reynolds number is 1000. Note that in this case, the diffusion process is no  
719 longer negligible in the chemical reaction. Concerning the forward problem,  
720 the velocity field is not altered by this modification. However, important  
721 changes are observed in the concentration field. The pressure drop ratio is  
722 important for this case, as can be seen from fig. 8, on the top left. This

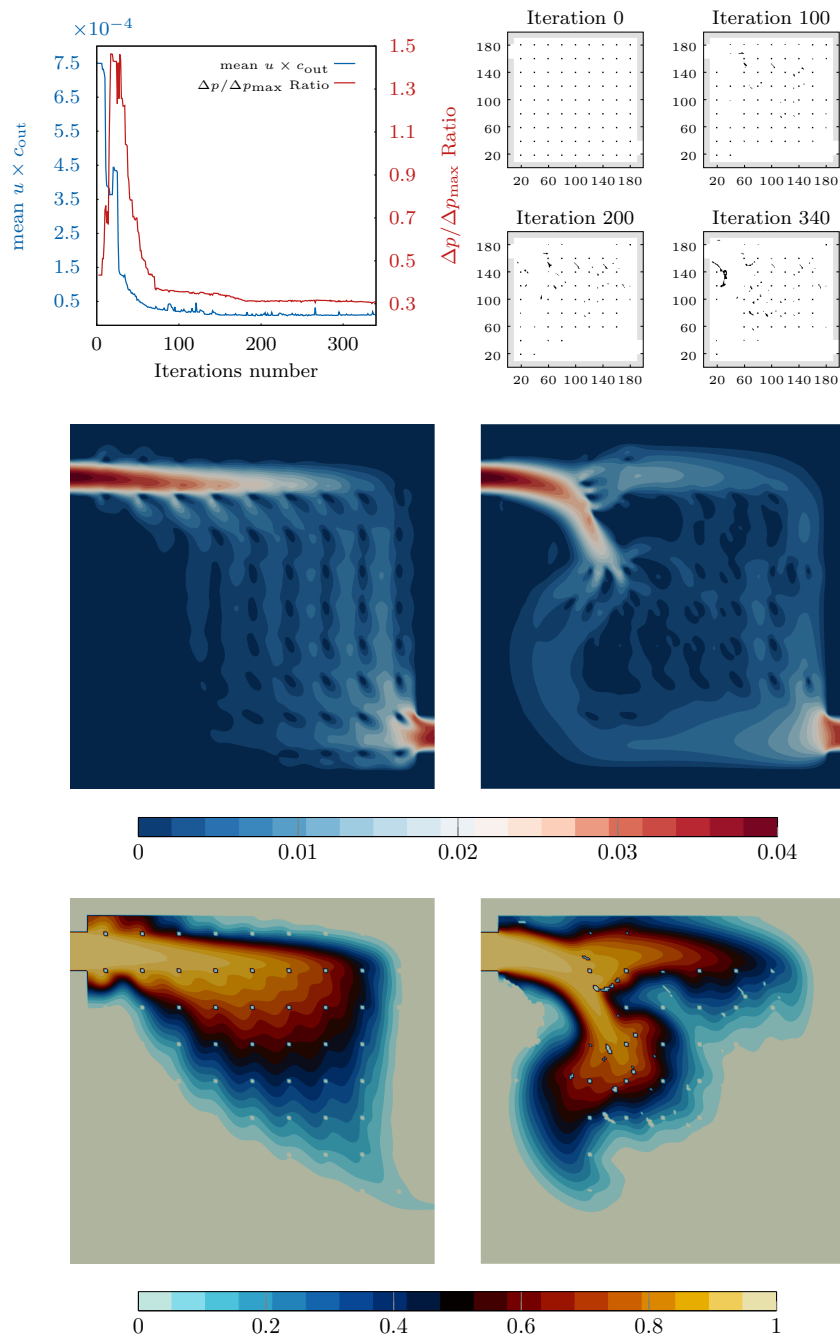


Figure 6:  $Da = 4 \times 10^{-5}$ . Top left: evolution of the cost function and of the pressure drop ratio along with the iteration count. Top right: the topology at iterations 0, 100, 200, and 340. Middle: module of the velocity field. Left: guess configuration (full fluid). Right: optimized topology. Bottom: concentration field. Left: guess configuration (full fluid). Right: optimized topology.

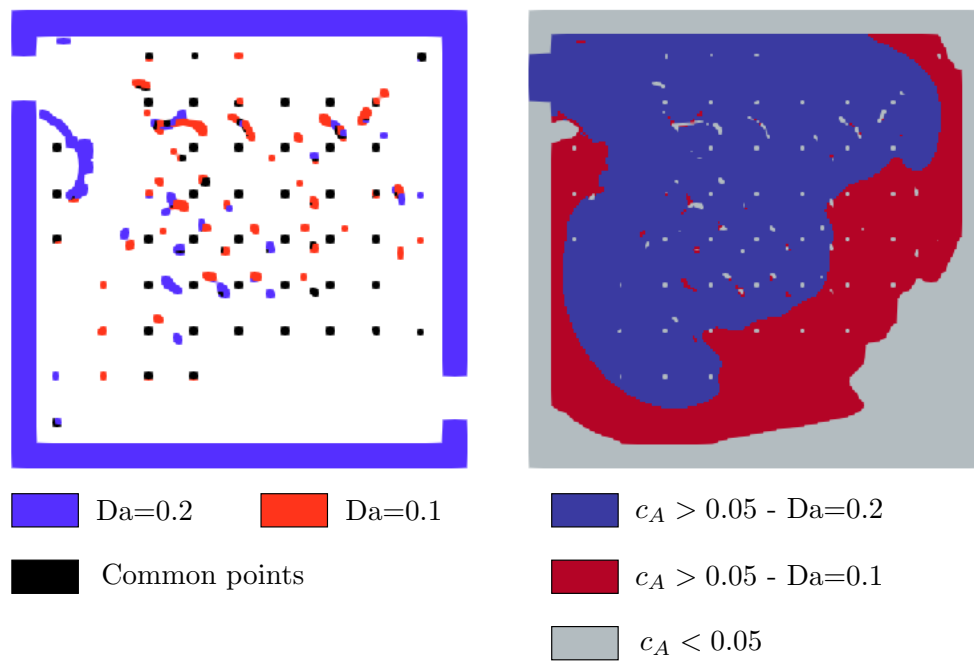


Figure 7: Comparison of optimization cases for  $Da=0.1$  and  $Da=0.2$ : optimal topologies (left) and concentration levels (right)

723 can be explained by the presence of solid parts near both the inlet and the  
724 outlet of the domain. Similarly to previous examples, the flow is divided into  
725 two paths near the inlet. With the initial topology, the reactant was spread  
726 from the inlet towards only the top-right corner of the domain. With the  
727 optimal topology, an equilibrium has been found between the propagation  
728 of the reactant on both the top-right corner and the bottom-left corner:  
729 a symmetry of the concentration can be observed, from the inlet down to  
730 the outlet. One can notice that, to obtain this behavior, the fluid flow is  
731 progressively divided into smaller channels from the inlet to the center of  
732 the domain. Indeed, the density of solid parts is the most important on the  
733 diagonal connecting the bottom-left corner to the top-right corner. With  
734 such a pattern, the minimization of the outlet concentration is well achieved.

#### 735 *5.4. Overview and analysis of the different results*

736 The characteristics of the optimized geometries obtained for all cases are  
737 summarized in table 2.

738 Among all cases, the decrease of the cost function is less important for  
739  $Re=10$  (case 1) and for  $Pe=100$  (case 5). In these two cases, either the  
740 advection is the smallest ( $Re=10$ , case 1), or the diffusion is the greatest  
741 ( $Pe=100$ , case 5), and the consequences are the same: the impact of the  
742 velocity field on the concentration is reduced, and so is the impact of the  
743 topology on the chemical reaction efficiency.

744 For the study on the Damkholer number, the reaction rate is multiplied  
745 by 2 (from the test case 3 to the test case 4), and the impact of this modifi-  
746 cation is consequent on the final value of the cost function. The initial value  
747 was also lower than the other cases, about one order of magnitude compared  
748 to the case 3. As it has been stated in section 5.2, the major conclusion  
749 regarding the optimized geometry obtained for this case is not only the effi-  
750 ciency of the reaction, but rather the over-sizing of the reactor. In fig. 7, one  
751 can see that there are less solid parts in the core of the domain for  $Da =0.2$   
752 than for  $Da =0.1$ . The porosity value in table 2 does not reflect this, but this  
753 can be explained by the fact that for  $Da =0.2$ , the biggest solid part (which  
754 is curved and close to the inlet) represents alone 0.37 % of the total porosity.

755 From table 2, it is seen that the pressure drop ratio slightly increases for  
756  $Re=10$  (case 1) and for  $Re=100$  (case 2), but this pressure drop decreases  
757 for  $Re=1000$  (case 3) and  $Da=0.2$  (case 4). In all cases, as the maximal  
758 pressure drop is prescribed to twice the pressure drop given for the initial  
759 geometry, the initial pressure drop ratio is equal to 0.5. So, for the two first

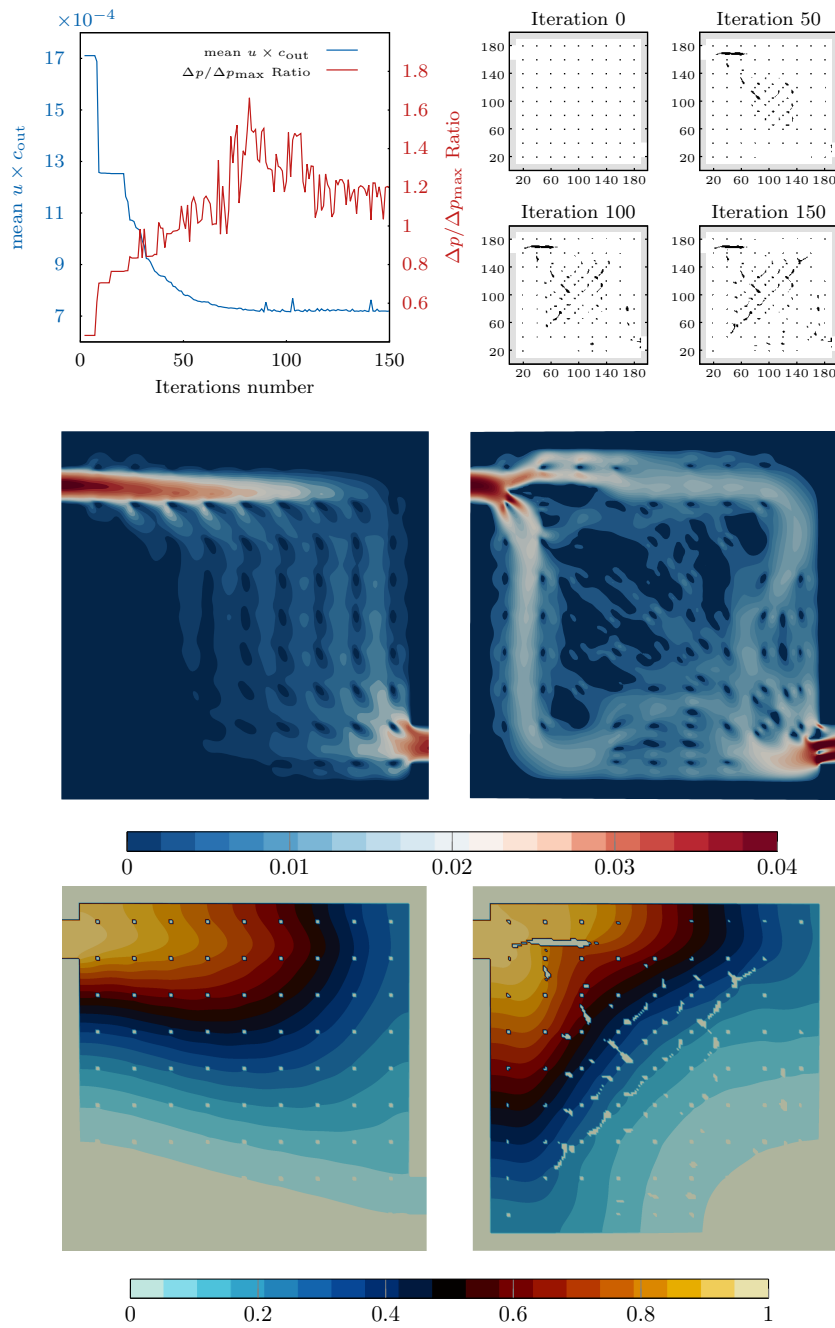


Figure 8:  $Pe=100$ . Top left: evolution of the cost function and of the pressure drop ratio along with the iteration count. Top right: the topology at iterations 0, 50, 100, and 150.

Middle: module of the velocity field. Left: guess configuration (full fluid). Right: optimized topology. Bottom: concentration field. Left: guess configuration (full fluid). Right: optimized topology.

760 cases, any added solid within the void medium would increase this pressure  
 761 drop ratio. However, as the initialization for  $Re=1000$  is realized with a  
 762 uniform distribution of small circles, the pressure drop can be smaller to the  
 763 initial one if some circles are removed, especially near the inlet and near  
 764 the outlet of the domain. This phenomenon happens for  $Re=1000$  (case 3)  
 765 and for  $Da=0.2$  (case 4). For the test case 5 (study on the Peclet number),  
 766 the initialization also involves circles, but, as some additional solid parts are  
 767 introduced, especially near the inlet and near the outlet, this participates to  
 768 an increase of the pressure drop ratio. As it can be seen on the different figures  
 769 concerning this study, the porosity for a lower Peclet number is higher than  
 770 for the other cases. The optimization domain is composed of more solid parts  
 771 to have a stronger control on the velocity field, useful to counter-balance the  
 772 higher diffusivity, but this is costly in term of pressure drop. One can notice  
 773 that in all the cases, the optimization process is achieved by the addition of  
 774 a small amount of materials (98.26 % of minimal final porosity, except for  
 775 the low Pe number test). This last configuration is characterized by a lower  
 776 porosity (97.1 %, which corresponds to three times more added material).  
 777 The term porosity not only explains the amount of material but also its  
 778 structure. Indeed, except at the lowest Re number, where optimal form acts  
 779 as a profile by splitting the initial major flow, the optimal solid distributions  
 780 look like porous media. In both the  $Re=100$  case and low Pe number case,  
 781 a plane structure appears in the diagonal of the cavity, perpendicular to the  
 782 line joining the entrance and the exit. This structure acts as a perforated  
 783 plane with adjusted holes in order to control and to balance the fluid flow.

784 In all these configurations, the optimization algorithm has been able to  
 785 design different topologies able to increase the efficiency of the chemical re-  
 786 actors, showing its adaptability and usefulness working with several physical  
 787 parameters involved in a multiphysics problem.

Case #	Da	Re	Pe	$\mathcal{J}^*$	$\mathcal{J}^{(0)}/\mathcal{J}^*$	$\Delta p$ ratio	Porosity
1	0.1	10	2000	1.9	2.60	0.53	98.72%
2	0.1	100	2000	0.59	10.40	0.61	98.26%
3	0.1	1000	2000	0.49	9.08	0.33	98.85%
4	0.2	1000	2000	0.012	62.50	0.306	98.75%
5	0.1	1000	100	0.72	2.36	1.03	97.1%

Table 2: Optimization results for different configurations

788 **6. Conclusion**

789 A topology optimization algorithm has been developed for advection-  
790 diffusion-reaction equations. The physical goal was the maximization of the  
791 reaction within the porous domain. This was measured through the mini-  
792 mization of the concentration flow out of the domain. The evolution of the  
793 topology was performed thanks to the evolution of a level-set function and  
794 a gradient-type method. Both the forward and the adjoint-state problems  
795 have been computed with the lattice Boltzmann method, with a passive scalar  
796 approach, and a reaction term for the modeling of the concentration field.  
797 Though the single-relaxation time collision operator was used for the concen-  
798 tration field, the flow field has been computed with the multi-relaxation time  
799 collision operator. This enabled computations with regimes up to  $Re=1,000$ .  
800 For both clarity and conciseness considerations, both forward and adjoint-  
801 state problems have been written down in residual forms.

802 The numerical applications enabled to exhibit strongly different behaviors  
803 with respect to the flow regime. Particularly, flows with  $Re=10$ ,  $Re=100$ ,  
804 and  $Re=1,000$  have been tested. For the specific case of  $Re=1,000$ , it has  
805 been shown that the presence of the recirculation zone went against a good  
806 convergence of the optimization process. As such, a modification of the initial  
807 guess topology, with the introduction of different small solid zones inside the  
808 medium, leads to a better convergence of the optimization problem.

809 Then, a study of the most important physical parameters (Damkholer and  
810 Peclet numbers) involved in the chemical reaction was done. As this prob-  
811 lem involves multiple coupled phenomena (advection, diffusion and reaction),  
812 their influence on the forward and optimization problem was important to  
813 be discussed. First, the reaction rate has been modified for the study on  
814 the Damkholer number. Even if the reactant was consumed faster, it was  
815 still possible for the algorithm to suggest an efficient design to minimize the  
816 cost function. Second, about the Peclet number, the choice was made for the  
817 first numerical examples to work with an advection-dominated problem, com-  
818 pared to mass diffusion, with a high Peclet number, in order for the velocity  
819 flow to have an important impact on the efficiency of the reaction. However,  
820 it was shown that the algorithm was also working fine with a lower Peclet  
821 number, where diffusion was not negligible anymore. In this case, a very reg-  
822 ular symmetry has been achieved by the optimized fluid/solid distribution,  
823 participating to a substantial decrease of the outlet concentration.

824 A crosscheck has also been performed in order to evaluate the results,



825 and enhance the reliability of the topology optimization method. Although  
826 a local minimum was found for  $Re=10$ , the comparisons with  $Re=100$  and  
827  $Re=1000$  has been successful as the best performance was achieved with the  
828 corresponding optimized geometry.

829 In further perspectives, the local minimum treatment is an interesting  
830 issue to solve, despite the fact that it can be difficult to avoid them while  
831 using a gradient-based optimization method. Nevertheless, one possibility  
832 would be to use a multi-scale resolution approach. Such a multi-resolution  
833 approach, formalized by Liu [67] for solving some ill-posed inverse problems,  
834 has been later on successfully used by Dubot et al. [68] and Liu [69], for  
835 example. In the framework of reactive fluid flow topology optimization, the  
836 use of a multi-scale resolution approach would enable to perform a scale-by-  
837 scale optimization on successive convex cost functions, following the work  
838 of Chavent [70]. Moreover, added to this interesting property, this would  
839 also save computational time due to faster convergence. This point will be  
840 addressed in a future research.

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