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# CFD modelling of axial mixing in the intermediate and final rinses of Cleaning-in-Place procedures of straight pipes

Jifeng Yang<sup>1</sup>, Bo Boye Busk Jensen<sup>2</sup>, Mikkel Nordkvist<sup>2</sup>, Peter Rasmussen<sup>3</sup>, Krist V Gernaey<sup>1</sup>, Ulrich Krühne<sup>1\*</sup>

<sup>1</sup> *Process and Systems Engineering Center (PROSYS), Department of Chemical and Biochemical Engineering, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark*

<sup>2</sup> *Alfa Laval Copenhagen A/S, 2860 Søborg, Denmark*

<sup>3</sup> *Carlsberg Danmark A/S, 7000 Fredericia, Denmark*

\*Correspondence to Ulrich Krühne, E-mail: [ulkr@kt.dtu.dk](mailto:ulkr@kt.dtu.dk), Tel: +45 4525 2960

Abstract:

The intermediate and final rinses of straight pipes, in which water replaces a cleaning agent of similar density and viscosity, are modelled using Computational Fluid Dynamic (CFD) methods. It is anticipated that the displacement process is achieved by convective and diffusive transport. The simulated agent concentrations show good agreement with the analytical axial mixing models from literature. The displacement time, minimum water consumption, minimum generation of wastewater and minimum requirement of intermediate rinsing water are evaluated using CFD. Practical empirical equations are derived from CFD results and applied to examine if the process is operated in an efficient and economic manner. It has been found that the displacement time can be predicted from the inner pipe diameter and the mean flow velocity using a power law relationship. Changing flow velocities does not significantly influence the minimum water consumption and the minimum wastewater generation for rinsing a pipe. Controlling the rinsing step based on a downstream measurement still consumes more water than the minimum requirement to reduce contamination risks. This article presents an innovative algorithm for optimizing the rinse steps with lower water consumption based on the above observations. A case of rinsing a 24 m long straight pipe describes the promising application of the CFD study. The recovery of cleaning agent can be up to 89.3% of the

25 volume and the saving of intermediate rinsing water can be at least 55% compared to the conventional  
26 rinse method. The work in this article presents an example showing how to deal with more complex  
27 systems in the future.

28 Keywords: Rinse; CFD; CIP; Axial mixing; Reducing water consumption

## 29 Nomenclature

$C_0$	Initial agent concentration, [kg m <sup>-3</sup> ]
$C_m$	Average agent concentration, [kg m <sup>-3</sup> ]
$C_\mu$	Model constant for solving the turbulence length scale and the dissipation rate of turbulence kinetic energy, dimensionless
$d$	Pipe diameter, [m]
$D_t$	Turbulent diffusivity of species, [m <sup>2</sup> s <sup>-1</sup> ]
$f$	Volume factor, dimensionless
$k$	Turbulence kinetic energy, [m <sup>2</sup> s <sup>-2</sup> ]
$K$	Axial dispersion coefficient, [m <sup>2</sup> s <sup>-1</sup> ]
$l$	Mixing length, [m]
$r$	Radial coordinate, [m]
$R$	Pipe radius, [m]
$t$	Time, [s]
$t_1$	The time required for displacing 1% of agent by water, [s]
$t_{99}$	The time required for displacing 99% of agent by water, [s]
$Ti$	Turbulence intensity, dimensionless
$Ti_b$	Turbulence intensity at inlet, dimensionless
$Tl$	Turbulence length scale, [m]
$Tl_b$	Turbulence length scale at inlet, [m]
$u_0$	Mean flow velocity, [m s <sup>-1</sup> ]
$u_x$	Axial flow velocity, [m s <sup>-1</sup> ]
$u'$	Fluctuating velocity, [m s <sup>-1</sup> ]

$V$	Pipe volume, [m <sup>3</sup> ]
$V_{inter. rinse}$	Volume of intermediate rinsing water, [m <sup>3</sup> ]
$V_{min}$	Minimum water consumption, [m <sup>3</sup> ]
$V_{wastewater}$	Volume of wastewater, [m <sup>3</sup> ]
$x$	Pipe length, [m]
$y^+$	Wall distance for a wall-bound flow, dimensionless
$\alpha, \beta$	Coefficients correlating the inner pipe diameter and the displacement time
$\varepsilon$	Dissipation rate of turbulence kinetic energy, [m <sup>2</sup> s <sup>-3</sup> ]
$\mu$	Dynamic viscosity, [Pa s]
$\rho$	Density, [kg m <sup>-3</sup> ]

## 30 Abbreviations

CFD	Computational Fluid Dynamics
CIP	Cleaning-in-place
DN	Nominal diameter
EHEDG	European Hygienic Engineering & Design Group
ERT	Electrical resistance tomography
RTD	Residence time distribution

31

32

## 33 1. Introduction

34 Cleaning-in-place (CIP) has become a common practice in food processing. The concept of CIP is to  
35 clean components of a plant or pipe without dismantling or opening the equipment and with little or no  
36 manual involvement of the operator (Lelieveld et al., 2005). In the food industry, CIP tends to consist  
37 of a series of similar steps, including: (1) *Product recovery* to drain the product from the system; (2)  
38 *Pre-rinse* for removing excessive soils from the system; (3) *Circulation of alkaline solution* to lift the  
39 soils from the plant surface and dissolve or suspend the soils in the detergent solution; (4)  
40 *Intermediate rinse* by water for removing the alkaline and entrained soils; (5) *Circulation of acid*  
41 *solution* to remove inorganic soils; (6) *Intermediate rinse* using water for removing acid; (7)  
42 *Disinfection (optional)* to eliminate microorganisms if a sanitary environment is required for the  
43 subsequent processes; (8) *Final rinse (optional)* to remove residual agents. If there is no disinfection  
44 step, the water quality in step 6 is often improved by treating with chlorine dioxide (Tamime, 2008).

45 In a recent mapping project performed at a leading brewery manufacturing site (Carlsberg Denmark),  
46 more than 33 CIP operations occur every day for cleaning tanks and pipes. Among these CIPs, pipe  
47 cleanings contribute with over 50% of the costs (Yang, 2017). Figure 1 (A) and (B) display the  
48 cleaning time of each step and the costs connected to a typical CIP of transfer pipes, respectively.  
49 Most of the cleaning time and costs are spent on alkaline/acid treatment, disinfection and the three  
50 rinsing steps (two intermediate rinses and one final rinse). The recovery of the cleaning detergents  
51 (alkaline and acid) can be up to 95% of the supply. In some industries, the final rinsing water can be  
52 partly recycled for the pre-rinse of the next CIP. The intermediate rinsing water is rarely recycled.  
53 Therefore, the overall recovery efficiency of rinsing water is very low, even less than 10%. Most of the  
54 rinsing water is directly disposed to drain.

55 Cleaning generates large amounts of wastewater containing corrosive pollutants, nutrients, and  
56 potentially a considerable organic load. Furthermore, heat losses due to discharge of hot water also  
57 contribute to the overall costs. Minimizing the environmental impact of cleaning has become more and  
58 more important due to the legislative pressures towards establishing zero emission processes  
59 (Palabiyik. 2013). A number of studies have focused on the development of new cleaning agents, the  
60 effect of water quality and the optimization of chemical usage (Chen et al., 2012; Jurado-Alameda et  
61 al., 2016; Palabiyik et al., 2015). However, industrial applications of such technologies are still limited  
62 due to the complex modification of existing equipment and the inestimable payback time. Operators  
63 tend to prefer simple changes in operation without significant transformation of the existing processes.  
64 Therefore, reducing the water consumption by optimizing flow rates and rinsing time in rinsing steps  
65 and improving the recovery efficiency of cleaning agent becomes a practical solution for many food  
66 industries, as the operators can easily change and dynamically adapt the flows at the control panel.

67 The rinsing objective is to displace residual cleaning agents (alkaline, acid and disinfectant) and  
68 reduce cross-contamination risks (Tamime, 2008). Such displacement of one liquid (chemical agent)  
69 with another liquid (water) occurs at the interface of two liquids, where an axial mixing zone is created  
70 due to convection and diffusion phenomena (Wiklund et al., 2010). The knowledge about axial mixing  
71 and the displacement zone is of importance in order to ensure complete chemical removal at reduced  
72 water consumption.

73 Computational fluid dynamics (CFD) methods are powerful in order to understand and predict fluid  
74 flows. A number of studies have applied CFD methods to understand how the local hydrodynamic  
75 conditions, e.g. shear stress and fluctuation intensity, affect cleaning results (Jensen et al., 2006;  
76 Jensen and Friis, 2005; Schöler et al., 2012) and to improve the hygienic design of valves, pipes and  
77 connections (Friis and Jensen, 2002; Jensen and Friis, 2004). Li et al. (2015a, 2015b) simulated a  
78 four-lobed swirl pipe by using CFD and identified the potential to improve the efficiency of CIP by



79 introducing swirl impact by increasing the local wall shear stress. CFD could also successfully predict  
80 the displacement of yoghurt by water, which agreed well with the measurement by using electrical  
81 resistance tomography (ERT) electrode planes (Henningsson et al., 2007).

82 Nearly all CFD studies applied to CIP considered water as the fluid to remove soils from the surfaces.  
83 There are, to our knowledge, no CFD investigations about the intermediate or final rinses where water  
84 is mainly used to displace cleaning agents. Compared with analytical mathematical models, the use of  
85 CFD models can get the information about mixing in both axial and radial directions. In some cases,  
86 CFD models can replace on-line measurement, as the installation of probes increases the capital cost  
87 and may introduce new areas that are difficult to clean. Moreover, CFD applies to complex geometries  
88 and is very helpful in the frame of hygienic design.

89 Pipe systems embrace several types of elements, e.g. straight pipes, bends, T-joints, expansions,  
90 contractions and valves. The cleaning difficulties vary depending on the design of these elements and  
91 the operation conditions. Investigating single and simple geometries is an important step if the  
92 complex geometries with various pipe elements are going to be studied. Therefore, the purpose of this  
93 paper is to simulate the axial mixing and the displacement phenomenon in the intermediate and final  
94 rinses of CIP procedures for straight pipes using CFD. The CFD results are validated using published  
95 empirical results based on an analytical mixing model for a turbulent flow regime in order to gain  
96 confidence in CFD for future studies of more complex systems. A detailed understanding of the axial  
97 mixing in CIP supports the knowledge about the effects of flow patterns on the process. The minimal  
98 time required to completely displace the residual agents can also be predicted. Furthermore, the total  
99 water consumption can be minimized by the proper combination of flow rate and rinsing time as well  
100 as by the implementation of efficient recovery plans.

101 2. Methods

102 This section describes two models: the first is the Taylor model, which provides an analytical solution  
 103 to describe the axial mixing of two fluids in a pipe; another is the CFD model, which is developed in  
 104 this study.

## 105 2.1. Taylor model

106 The Taylor model (in equation 1) describes the axial dispersion of steady incompressible Newtonian  
 107 fluids flowing in the laminar regime. The model has then been extended to cover non-Newtonian fluids  
 108 and turbulent flows (Levenspiel, 1958; Zhao et al., 2010):

$$C_m = \frac{C_0}{2} \left( 1 - \operatorname{erf} \left( \frac{x - u_0 t}{2\sqrt{Kt}} \right) \right) \quad (1)$$

109 where  $C_m$  is the average agent concentration at length  $x$  and time  $t$ ,  $C_0$  is the initial agent  
 110 concentration,  $u_0$  is the mean flow velocity,  $K$  is the axial dispersion coefficient,  $\operatorname{erf}$  is the error  
 111 function. In the process of water displacing cleaning solutions in a pipe, the boundary conditions are

$$\begin{aligned} \text{when } t = 0, C = C_0 \text{ at } x \geq 0 \\ \text{when } t > 0, C = 0 \text{ at } x = 0 \end{aligned} \quad (2)$$

112 The empirical correlation of the axial dispersion coefficient for turbulent flows based on experimental  
 113 measurements,  $K$ , is according to *Salmi et al.* (2010):

$$\frac{K}{u_0 d} = \frac{3 \times 10^7}{Re^{2.1}} + \frac{1.35}{Re^{0.125}} \quad (3)$$

114 where  $u_0$  is the mean flow velocity,  $d$  is the inner pipe diameter,  $Re = du_0\rho/\mu$  is the Reynolds number.  
 115 Under the studied flow conditions, which are described later, the second term on the right hand side in  
 116 equation 3 dominates the value of  $K$ . So the dependency of  $K$  on  $u_0 d$  can also be approximated by a  
 117 correlation of  $(u_0 d)^{7/8}$ .

## 118 2.2. CFD simulation

## 119 2.2.1. Flow domain and mesh

120 A series of horizontal straight pipes of 28 m in length were simulated. The inner diameters of the pipes  
121 were 15.80, 26.64, 40.90, 77.90 and 154.10 mm respectively, in accordance with the European pipe  
122 size standards of DN 15, 25, 40, 80 and 150 mm with the pipe wall thickness defined by the standard  
123 pipe schedule. The surface boundaries were modelled as smooth, which is required for food  
124 processing.

125 The geometries were simplified to be quarter sections, as the flow profiles were symmetric along the  
126 radial direction. Such a simplification reduced the computational time significantly compared with the  
127 simulation of the whole pipe geometry. It also retained cuboid mesh elements at the center of the  
128 pipes. Structured hexahedral meshes were made with help of the meshing software ANSYS ICEM  
129 CFD 16.2. A mesh independence test was carried out and described in section 2.2.3 (comparing  
130 cases 2, 6 and 7) in order to minimize the errors associated with the mesh size. The mesh layers in  
131 the near-wall regions were enhanced to capture the flow details close to the wall (Figure 2). The  
132 resulting meshes had a fixed number of nodes in the axial direction (501 nodes) and varying numbers  
133 of layer nodes in the radial direction. The attained values of  $y^+$ , the dimensionless distance from the  
134 wall, are 27 – 67. The total number of mesh elements was 37650, 72794, 180646, 663646 and  
135 2098360 respectively, contributing to a mesh density of 450 – 770 elements/mL.

## 136 2.2.2. CFD model description

137 Water and the agent solutions are miscible. The properties of the agent solution (i.e. density and  
138 viscosity) were assumed to be the same as water. Therefore, a single liquid phase simulation was  
139 made in this study.

140 First, a steady state simulation was performed using water to obtain the flow profiles. The inlet was set  
141 as plug flow with the mean flow velocities of 1.0, 1.5 and 2.0 m/s, corresponding to the standard

142 working velocity range in industrial practices (Chisti and Moo-Young, 1994). The outlet was defined  
143 with a relative pressure of 0 Pa. The Reynolds numbers were calculated to be above 17000. Thus, all  
144 the flows were fully turbulent. The effects of turbulence intensity ( $Ti$ ) and turbulence length scale ( $l$ )  
145 at the inlet boundary are presented in section 2.2.3 (comparing cases 1 - 5).

146 Subsequently, a transient simulation was performed using the steady results as initial conditions. The  
147 pipe was divided into two sections in order to eliminate the entrance effects under which the flow was  
148 not fully developed. It was crucial to introduce this additional length of the pipe, since a boundary  
149 condition at the inlet was chosen, where at any point of the inlet the same velocity was defined.  
150 Therefore, a certain length was needed, before the correct velocities in radial direction were  
151 established as shown in Figure 3. The first section was  $-3 \leq x < 0$  m, where water was flushed from  
152  $t = 0$  and contacted with the agent solution at  $x \geq 0$  m. The second section was  $0 \leq x \leq 25$  m, where  
153 the cleaning agent components were dissolved in water with an initial concentration of  $1 \text{ kg/m}^3$ . The  
154 agent component was expressed as an additional volumetric variable, which could be transported  
155 through the flow via diffusion and convection (ANSYS CFX-Solver Theory Guide, ANSYS INC, 2013).

156 Buoyancy was not taken into account, because it has been tested that buoyancy did not contribute  
157 much to axial mixing, especially when there was no density difference between the two fluids (Zhao et  
158 al., 2010). The axial dispersion coefficients were determined with help of equation 3. In the studied  
159 flow conditions, the  $K$  values range from  $0.006 - 0.08 \text{ m}^2/\text{s}$  and the second term on the right hand  
160 side in equation 3 contributes with over 90% to calculation of the  $K$  value.

161 The model was built with help of ANSYS CFX version 16.2 using the standard  $k - \varepsilon$  turbulence model  
162 with scalable wall functions. The advection scheme was set to be high resolution. Steady state  
163 simulations in the CFX software are pseudo transient simulations, where also a timescale has to be  
164 defined. This can be done automatically, which was our approach, or otherwise a time step has to be

165 defined (physical timescale). For the here presented steady state simulations, the timescale was  
166 automatically controlled by the CFX-Solver software (auto timescale) to 0.032 s ~ 0.15 s. The  
167 iterations were forced to run for minimum 500 steps, even though the convergence criteria (residual  
168 target  $MAX \leq 0.00001$ ) had been reached after ~100 steps. For the transient simulations, the Courant  
169 number is of fundamental importance to reflect the part of a mesh element that a solute will traverse  
170 by advection in a time step. The definition is the product of the local velocity and the time step, divided  
171 by the mesh element characteristic length. In the simulations, the time step was 0.01 s, corresponding  
172 to the maximum Courant number of 0.42 – 0.92 for different pipe diameters and flow velocities.

### 173 2.2.3. Mesh independence test and inlet boundary conditions

174 Table 1 shows 7 cases of simulations which were carried out to minimize the errors associated with  
175 the mesh size and flow inlet conditions. The mesh study was performed by refining the mesh in single  
176 radial direction (case 7) or in both radial and axial directions (case 6), and comparing the turbulence  
177 intensity near the wall and the average agent concentrations at different distances with the reference  
178 case 2. All the studies were performed based on the inner pipe diameter of 40.90 mm (DN 40) and a  
179 flow velocity of 1.5 m/s.

180 In addition to the flow velocity, the turbulence at the inlet is defined by the turbulence intensity ( $Ti$ ) and  
181 the turbulence length scale ( $Tl$ ) (Wilcox, 2006). In this study, the turbulence magnitude of the inlet was  
182 studied by comparing cases 1 - 5 in Table 1, with changing turbulence intensity (1 – 20%) and  
183 turbulence length scale (5 – 30% of the pipe diameter). This approach was similar to the study of the  
184 influence of turbulence intensity at the inlet on wall shear stress fluctuations by Jensen (2007). Based  
185 on the results of the near-wall turbulence intensity in the steady state simulations and the predicted  
186 agent concentration at fixed planes in the transient simulations, the selected inlet boundary conditions  
187 for the final model were  $Ti = 5\%$  and  $Tl = 10\%$  of the pipe diameter.

## 188 3. Results and discussions

## 189 3.1. Studies of mesh independence and inlet boundary conditions

190 The predicted near-wall turbulence intensity initially drops, then rises, and reaches a uniform constant  
191 value ( $\sim 0.056$ ) apart from the pipe section covering the first 2 m after the entrance (as shown in  
192 Figure 4). Comparing cases 6 & 7 with case 2, finer meshes in radial and axial directions lead to a  
193 larger turbulence intensity in the turbulent section, but the change is less than 1% of deviation.  
194 Therefore, the differences caused by mesh sizes as well as the turbulence intensity and turbulence  
195 length scale are only limited to the initial 2 m pipe section.

196 Equation 1 indicates that  $C_m = C_0/2$  at the mid-plane, which is defined as the plane where the front of  
197 the water phase arrives when an ideal plug flow is assumed ( $x = u_0 t$ ). Figure 5 illustrates the average  
198 agent concentrations at four mid-planes (1.5 m, 9 m, 15 m and 21 m) simulated for the 7 model cases.  
199 It is found that all of the predicted values of  $C_m$  are lower than the theoretical value, which is mostly  
200 caused by the discretization error when a fluid domain is subdivided into a mesh. However, all of the  
201 deviations are less than 1% of the theoretical value calculated by equation 1. In particular, cases 1 - 5  
202 result in the same average agent concentration values (with precision  $0.00001 \text{ kg/m}^3$ ) at the four mid-  
203 planes. This observation strengthens the conclusion drawn from Figure 4 that the turbulence intensity  
204 and turbulence length scale of the inlet only affect the flow and mixing near the entrance, but no longer  
205 at  $x = 0$ .

206 Hence, if the analysis omits the entrance section, the mesh refinement, as presented for the cases 6  
207 and 7, is not necessary. Case 2 provides a sufficient mesh for this project. Extremely fine meshes may  
208 be counterproductive, because the mixing in radial direction is not significant (consider also Figure 9)  
209 and flat mesh elements lead to low mesh quality in slender pipes. The results imply that the use of 3 m  
210 pipe as entrance, as illustrated in Figure 3, is a reasonable measure to overcome the effects of

211 entrance fluctuations. The meshes of other pipe diameters were made by fixing axial nodes similar to  
212 case 2 and adjusting radial nodes to result in identical layer size and  $y^+$ . The inlet boundary conditions  
213 are selected to  $Ti = 5\%$  and  $Tl = 10\%$  of the pipe diameter. When a new mesh and a new flow  
214 velocity were employed, the same validation approaches as demonstrated in Figure 4 and Figure 5  
215 were carried out in order to ensure that the flow was in a turbulent condition at  $x = 0\text{ m}$  and  $C_m \approx$   
216  $0.5 C_0$  at the mid-planes.

### 217 3.2. Comparison of the Taylor model with CFD simulations

218 Figure 6 shows the agent concentrations at the mean flow velocity of 1.5 m/s at  $x = 15\text{ m}$  and for a  
219 fixed rinsing time (10 s) at an arbitrary distance. The presented values in Figure 6 are obtained from  
220 the calculations by the Taylor model (Taylor, 1953) and the CFD simulations. Figure 6(A) can be  
221 regarded as the displacement dynamics at the fixed plane during the rinsing period. Figure 6(B) can  
222 be regarded as the agent distributions within the pipe after 10 s of rinsing.

223 The agent components transfer slower near the wall than in the center due to blunt velocity profiles  
224 (Figure 7). The longer tails in larger pipes (Figure 6) indicate that the agent components are axially  
225 mixed faster in the pipe center but slower near the wall than in smaller pipes. The mixing of agent  
226 molecules is a result of convection and diffusion (Wiklund et al., 2010). According to equation 3, the  
227 value of the axial dispersion coefficient increases with increasing pipe diameter when the flow is  
228 turbulent (Salmi et al., 2010). In Figure 7, the value of  $k$  is minimal at the center and increases towards  
229 the radial direction, and decreases near the wall, which is the same as Zhao et al. (2010) observed  
230 when simulating the mixing of two miscible liquids with different densities. Considering the velocity of  
231 the largest pipe at the center is  $\sim 3\%$  lower than the smallest pipe, it can be concluded that the mixing  
232 of the agent component is governed by axial diffusion in the pipe center section, and by convection  
233 near the wall.

234 CFD successfully predicts the values which are calculated with help of the Taylor model (Taylor, 1953).  
235 The model therewith predicts accurately the analytical model in terms of the transient agent  
236 concentrations at different locations in the pipe. In addition to the Taylor model, the prediction of  
237 dispersion within a pipe by using CFD has also been verified to be successful by predicting Sugiharto  
238 et al. (2013)'s experimental data and the residence time distribution (RTD) theory (Bailey and Ollis,  
239 1986). The validations of the latter two approaches are provided in supplementary materials.  
240 Therefore, the CFD model is used for further investigations of the displacement process and the  
241 mixing zone analysis.

### 242 3.3. Displacement time

243 Three displacement times are defined in this work for different purposes:

- 244 •  $t_{1,plane}$  is the time when 1% of the agent is displaced by water at a fixed plane ( $C_m = 0.99 C_0$ ).  
245 It is assumed to be the detected start point of rinsing when measurements are employed to  
246 determine the agent concentration. The sensor is located at the flow downstream from where  
247 the plane lies;
- 248 •  $t_{99,plane}$  is the minimum rinsing time to remove 99% of the agent component at the fixed plane  
249 ( $C_m = 0.01 C_0$ ). In practice, it is the apparent time where rinsing ends once the downstream  
250 measurement outputs reach the pre-defined rinsing criteria;
- 251 •  $t_{99,volume}$  is the minimum rinsing time to remove 99% of the cleaning agent from the volume,  
252 which is the true time required to replace the agent component and reduce contamination risks.

253 The selection of 99% as complete rinsing refers to Graßhoff's (1983) work when studying the  
254 displacement of one liquid with another liquid during CIP. Depending on the initial agent concentration  
255 and the requirement of cleaning in different industries, the minimum rinsing time may be defined to  
256 remove more or less than 99% of cleaning agent in order to achieve a safe level.



257 It is observed that the product of the displacement time and the mean flow velocity,  $t_{1\ or\ 99} \cdot u_0$ , is  
 258 constant for different flow velocities, which can be correlated by a power function like equation 4 with  
 259 the inner pipe diameter as variable. Figure 8 illustrates  $t_{1\ or\ 99} \cdot u_0$  against the inner pipe diameter at  
 260 different length of pipe sections. The values of the correlation parameters for three pipe lengths (2, 15  
 261 and 24 m) are presented in Table 2. The small values of  $\beta$  indicate that the rinsing times are mainly  
 262 influenced by the flow velocity and pipe length, instead of the pipe diameter. In a CIP rinse, such  
 263 correlations help to make predictions about when the recovery of agent should be stopped and when  
 264 the recovery of rinsing water should be launched.

$$t_{1\ or\ 99} \cdot u_0 = \alpha \cdot d^\beta \quad (4)$$

265 An increase in pipe diameter not only speeds up the start of displacement, but also prolongs the  
 266 termination of displacement. It is caused by the longer tailing distribution of agent components in  
 267 larger pipes as described in Figure 6, which is observed in both CFD and Taylor models. The obtained  
 268 minimum rinsing time values based on the fixed plane are greater than the values based on the  
 269 volume. It can be understood in such a way that when 99% of the cleaning agent is removed from the  
 270 volume, the volume-weighted average agent concentration is 1% of the initial concentration.  
 271 Meanwhile, agent concentrations near the inlet are lower than near the outlet. So the average agent  
 272 concentration at the outlet plane is still above 1% at  $t_{99, volume}$ . In practice, the rinsing time can be  
 273 determined by measuring the agent concentration downstream and rinsing stops exactly when the  
 274 agent concentration reaches the pre-defined criteria. However, the apparent rinsing time in such a  
 275 situation is still longer than the true requirement in order to reduce contamination risks.

#### 276 3.4. Minimum water consumption for rinsing

277 The minimum water consumption for an effective rinsing is the minimum requirement of water to  
 278 reduce the amount of agent to such a low degree that the residues have no or only a minor effect on

279 the following steps. In this study, the removal of 99% of agent components is assumed as a complete  
 280 rinse. In order to compare the minimum consumption for different pipe diameters, a volume factor,  $f$ ,  
 281 is defined as the ratio between the minimum water consumption,  $V_{min}$ , and the pipe volume,  $V$ , as  
 282 follows:

$$f = \frac{V_{min}}{V} = \frac{\pi d^2/4 \cdot u_0 \cdot t_{min}}{\pi d^2/4 \cdot x} = \frac{u_0 \cdot t_{99}}{x} \quad (5)$$

283 Equation 4 indicates that the value of  $u_0 \cdot t_{99}$  only depends on the inner pipe diameter for a given pipe  
 284 length. Therefore, according to equation 5, the values of volume factors are independent of flow  
 285 velocities as well. The increase in flow velocity reduces the cleaning time significantly, but it does not  
 286 affect the minimum water consumption. However, if water also works as a medium to remove soils  
 287 from surfaces, large flow velocities improve cleaning efficiency by destroying the structure between  
 288 soils and surfaces by mechanical forces, i.e. shear stress (Tamime, 2008). The pipes of larger size  
 289 lead to larger volume factors, as  $t_{99}$  increases with increasing inner pipe diameters. Both the  
 290 numerator and denominator in equation 5 increase for longer pipes, but the value of  $u_0 \cdot t_{99}$  grows  
 291 slower than  $x$ . Thus, the volume factors become smaller for longer pipes.

292 With decreasing pipe diameter and increasing pipe length, the volume factor values tend to the lower  
 293 limit of 1, indicating that the minimum water consumption approaches the pipe volume. It can also be  
 294 concluded that the calculated volume factors based on the downstream measurement are larger than  
 295 the values based on the volume, which is the same trend as the illustrated cleaning time in Figure 8.  
 296 Therefore, if the cleaning time is controlled by downstream measurements, the consumption of water  
 297 is still 6 - 20% more than the real demand to remove a certain amount of agent from the volume.

298 3.5. Minimum volume of wastewater

299 Recovering of cleaning agent and rinsing water is an efficient solution to reduce the cleaning cost. For  
 300 a given pipe length, the recovery plan can be made in the following way:

- 301 • The recovery of cleaning agent stops at  $t_{1,plane}$ . So the agent solution is still in high  
 302 concentration without dilution and can be reused with high activity.
- 303 • The recovery of rinsing water starts at  $t_{99,plane}$ , as the rinsing water is less “polluted” by the  
 304 agent components. The recovered water can be used for the pre-rinse of the next cleaning or  
 305 for other applications where the water quality fits.
- 306 • The effluent between  $t_{1,plane}$  and  $t_{99,plane}$  is a mixture of the agent solution and the rinsing  
 307 water, which can be disposed to the drain or a wastewater treatment plant. The amount of  
 308 effluent can be regarded as the minimum amount of wastewater when the recovery is planned  
 309 according to this approach.

310 The minimum volume of wastewater is:

$$V_{wastewater} = \frac{\pi d^2}{4} \cdot u_0 \cdot t_{99,plane} - \frac{\pi d^2}{4} \cdot u_0 \cdot t_{1,plane} = \frac{\pi d^2}{4} \cdot (u_0 \cdot t_{99,plane} - u_0 \cdot t_{1,plane}) \quad (6)$$

311 As indicated by equation 4, the values of  $u_0 \cdot t_{99,plane}$  and  $u_0 \cdot t_{1,plane}$  only depend on the inner pipe  
 312 diameter for a given pipe length. Therefore, the minimum volume of wastewater increases as well  
 313 when the pipe diameter increases.

### 314 3.6. Mixing zone length

315 Figure 9 shows the process when the agent is displaced by water in a 1 m pipe section within 2 s. The  
 316 displacement occurs mainly in the axial direction. Mixing in radial direction is not significant when the  
 317 flow is in turbulent regimes (Chisti and Moo-Young, 1994). In this study, mixing length is defined as  
 318 the distance from the leading edge where the agent concentration is 99% to the trailing edge where  
 319 the agent concentration is 1%.

320 The study of mixing length is important for intermediate rinses, especially for long pipes. The usual  
321 practice is to completely displace the cleaning agent A by water before introducing another cleaning  
322 agent B. An alternative method is shown in Figure 10. Two cleaning agents can be synchronously  
323 introduced with a proper interval between the agents. A so called intermediate rinse length is the sum  
324 of the mixing zone length of the agent A, the mixing zone length of the agent B and an intermediate  
325 length between two mixing zones. The intermediate length between two mixing zones can be  
326 minimized in order to reduce water consumption. Thus, the minimum requirement of intermediate  
327 rinsing water is the volume of two mixing zones which can be calculated from the mixing length.

328 Figure 11 demonstrates that the mixing length increases continuously with increasing rinsing time. The  
329 leading edge (above 0) and trailing edge (below 0) are symmetrically located on two sides of the mid-  
330 plane. Zhao et al. (2010) also observed that the increase in flow velocities contributed to greater  
331 mixing lengths when simulating the displacement of a heavier liquid A with another lighter liquid B in a  
332 10 m straight pipe.

333 According to the penetration theory of Higbie (1935), the mixing length of different species is  
334 dependent upon both the turbulent diffusivity and the contact time (van Elk et al., 2007; Zhao et al.,  
335 2010):

$$l \propto 2\sqrt{D_t \cdot t} \quad (7)$$

336 where  $l$  is the mixing length,  $D_t$  is the turbulent diffusivity of the species. The right hand side term,  
337  $2\sqrt{D_t \cdot t}$ , is called characteristic length in mixing (Ekambara and Joshi, 2004). By replacing the  
338 turbulent diffusivity with the axial dispersion coefficient, equation 7 also applies to the axial mixing of  
339 CFD results as shown in Figure 12. The idea behind the correlation is that the penetration theory  
340 quantifies the component transfer using a similar error function as in equation 1 (Assar et al., 2014).

341 On the basis of the correlation, it enables to predict the mixing lengths for longer rinsing time and  
 342 various flow rates and pipe diameters.

343 For a given pipe length, the contacting time can be assumed as  $x/u_0$ , which is the mean residence  
 344 time of rinsing water. Then the minimum requirement of intermediate rinsing water can be calculated  
 345 from the mixing length, as:

$$V_{inter. \ rinse} = 2 \cdot \frac{\pi d^2}{4} \cdot l = 2 \cdot \frac{\pi d^2}{4} \cdot 3.29 \cdot \left(2\sqrt{K \cdot x/u_0}\right) = 3.29\pi d^2 \sqrt{K \cdot x/u_0} \quad (8)$$

346 Under the flow conditions in this study, the second right hand side term in equation 3 dominates the  
 347 value of  $K$ . Therefore, equation 8 can be further simplified and approximated as:

$$\begin{aligned} V_{inter. \ rinse} &= 3.29\pi d^2 \sqrt{1.35(u_0 d)^{0.875} (\mu/\rho)^{0.125} \cdot x/u_0} \\ &= 3.82\pi \sqrt{u_0^{0.375} d^{4.875} (\mu/\rho)^{0.125} x} \end{aligned} \quad (9)$$

#### 348 4. Application and further perspectives

##### 349 4.1. Understand and control the process

350 The objective of any rinsing operation should be to completely remove the cleaning agent solution  
 351 using less water, shorter time and generating less wastewater. With this purpose in mind, the obtained  
 352 knowledge from this study can be categorized into two groups: the first type of knowledge is about  
 353 controlling the process, including the flow velocity, the minimum rinsing time and the times for  
 354 recovering the cleaning agent or rinsing water; the second type of knowledge is about understanding  
 355 the process, like the minimum water consumption, the minimum volume of wastewater, the recovered  
 356 volume of the cleaning agent and the minimum requirements of intermediate rinsing water.

357 Figure 13 presents an algorithm flowchart about how to apply the existing complex knowledge to  
 358 optimization of the rinsing process. Given the pipe diameter, flow velocity and pipe length, the  
 359 minimum rinsing time can be calculated. In practical cases, the real rinsing time is normally set with

360 safety margins, as it is not desired to risk producing inferior products due to unwise savings in  
361 cleaning procedures. However, if the input rinsing time is much longer than the minimum required time,  
362 it should be examined if an unnecessary waste of time and water is the case.

363 It is expensive to run CFD simulation for all conditions. But using the empirical or analytical equations  
364 derived from CFD results is practical. Equation 4 calculates the time to stop the recovery of cleaning  
365 agent and the time to start the recovery of rinsing water. Correspondingly, the effluent between the  
366 two time points is regarded as wastewater, the minimum volume of which can be predicted with help  
367 of equation 6. If the real volume of wastewater is more than the minimum, it means the recovery  
368 efficiency can be higher by adjusting the recovery time. On the contrary, if the volume of wastewater is  
369 less than the minimum, it leads to the potential risk of excessive recovery. For example, the recovered  
370 cleaning agent has been diluted by the rinsing water, or the reused rinsing water has been “polluted”  
371 by the cleaning agent. If it is the intermediate rinse between two cleaning agent solutions, the  
372 minimum volume of intermediate rinsing water can be calculated according to equation 8 or 9.

373 4.2. A case study of rinsing a 24 m straight pipe with inner diameter 100 mm

374 The above results are extended to analyze the rinse of a 24 m straight pipe with inner diameter 100  
375 mm. The mean flow velocity is 1 - 2 m/s. The set time of the rinsing step is assumed to be  $1.5 \cdot x/u_0$ .  
376 In industrial practice, the rinsing time is usually set based on experience, which can thus be over or  
377 below 1.5 times the residence time. The density and dynamic viscosity are assumed to be  $997 \text{ kg/m}^3$   
378 and  $8.899 \times 10^{-4} \text{ kg/(m}\cdot\text{s)}$ , and are assumed the same for the agent solution and the rinsing water.

379 Table 3 summarizes the results, which have been produced using the algorithm summarized in Figure  
380 13. The calculated minimum rinsing time based on a fixed plane is 11.2% larger than the minimum  
381 rinsing time calculated based on the volume. The set time is 1.36 times the  $t_{99,volume}$ . The increase in  
382 flow velocity can shorten the rinsing time. However, the consumption of rinsing water, the recovery of

383 cleaning agent and the generation of wastewater are independent of the flow velocities. The recovery  
384 of cleaning agent is up to 89.3% of the volume. If it is the intermediate rinse, the increase in flow  
385 velocity slightly reduces the minimum requirement of intermediate rinsing water. An important result is  
386 that the implementation of synchronous intermediate rinse saves ~55% of water compared with the  
387 minimum requirement to replace all agent components from the pipe.

#### 388 4.3. Effects of complex element geometries

389 This study simulates the displacement process in straight pipes. However, a complete transfer line  
390 consists of various elements, such as bends, T-joints, expansions, contractions and valves. Graßhoff  
391 (1983) studied the displacement of one liquid with another liquid in three types of T-joints: (1) direct  
392 entrance and exit with a perpendicular dead zone; (2) perpendicular entrance and exit with the dead  
393 zone extending the entrance stream; and, (3) perpendicular entrance and exit with the dead zone  
394 reversing the exit stream. A local sensor was installed at the end of the dead zone. With the increase  
395 in the dead zone length from  $d$  to  $10d$ , the displacement time ( $t_{99}$ ) determined by the local sensor  
396 varied from seconds to ten thousands of seconds. Thus, the time to completely remove the cleaning  
397 agent from a long dead zone is much longer than for rinsing straight pipes.

398 CFD is a powerful tool to study the hygienic design of such elements. According to the European  
399 Hygienic Engineering & Design Group (EHEDG) Testing and Certification guideline, CFD is currently  
400 the only alternative to test the scalability of difference sizes of the same piece of equipment, apart  
401 from the evaluation based on a design review and CIP test (EHEDG.org, 2016). CFD simulations of  
402 the intermediate and final rinses serve as a supplement to previous studies where water is applied as  
403 a medium to dissolve or remove soils from the surfaces (Asteriadou et al., 2009, 2007, 2006). This  
404 article boosts the confidence to implement such CFD simulations of the displacement process for  
405 more complex element geometries which are more commonly used in practice.

## 406 5. Conclusions

407 In this paper, CFD is used to simulate the intermediate and final rinses of straight horizontal pipes in  
408 CIP applications. Axial mixing and displacement of agent solutions by water are studied and compared  
409 with the Taylor model. The proposed CFD model for description of agent concentrations at varying  
410 time points and locations in the pipe is found to give an excellent agreement with the Taylor analytical  
411 model.

412 The key findings in the presented work are summarized in the following:

- 413 1) The displacement times are dependent on the pipe diameters and flow velocities. The product  
414 of the displacement time and the mean flow velocity can be correlated by a power function with  
415 inner pipe diameter as independent variable.
- 416 2) The minimum water consumption for completely rinsing a pipe is slightly larger than the pipe  
417 volume. The minimum water consumption is not much influenced by changing flow velocities  
418 when the flows are fully turbulent.
- 419 3) A practical rinsing step can be controlled based on downstream measurement and rinsing  
420 stops when the measurement reaches the pre-defined criteria. However, the set time is still  
421 longer than required. The water consumption is still more than the minimum requirement in  
422 order to reduce contamination risks.
- 423 4) The minimum volume of wastewater can be predicted from the displacement times, and is  
424 independent of the flow velocity.
- 425 5) Radial mixing is not significant during the displacement process. The mixing length varies with  
426 the pipe diameters, flow velocities and rinsing time. The values of the mixing lengths are  
427 proportional to the characteristic length ( $2\sqrt{K \cdot t}$ ), which can be applied to calculate the  
428 minimum requirement of intermediate rinsing water.



429 The observations in this work can help to optimize the control of the rinsing step in terms of the flow  
430 velocity, the rinsing time and the recovery plans of the cleaning agent and rinsing water. A case study  
431 of rinsing a 24 m straight pipe with inner diameter 100 mm reveals that the recovery of cleaning agent  
432 can be up to 89.3% of the volume and the saving of intermediate rinsing water can be at least 55%.  
433 The successful simulation of the intermediate and final rinses of straight pipes builds confidence for  
434 future studies to simulate the displacement process for more complex geometries and improve the  
435 hygienic design and the CIP cleaning of different pipe elements.

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- 526

**Figure captions:**

Figure 1. (A) The cleaning time of each step and (B) the costs in a CIP procedure of transfer pipes in a brewery. The cleaning is performed at room temperature. The recovery ( $\sim 95\%$ ) of cleaning chemicals has been considered in the calculation of the costs. (Reproduced with permission of Carlsberg, Fredericia, Denmark)

Figure 2. Structured mesh of the cross section of the pipe with diameter 40.90 mm (DN 40). The near-wall meshes were enhanced by fine layers. The geometry was simplified as a quarter section of the pipe in order to save computational time. The mesh element in the pipe center (at the bottom-left corner) was nearly cuboid.

Figure 3. Description of the distribution of agent component within the pipe at  $t = 0$ . The agent components were dissolved in water with a concentration of  $1 \text{ kg/m}^3$  at  $x \geq 0 \text{ m}$ . Water was flushed from  $x = -3 \text{ m}$ . Such treatment eliminated the entrance effect at  $x = 0$  under which the inlet flow was not fully turbulent.

Figure 4. Near-wall turbulence intensity (1 mm from the wall) for different model cases. The inner pipe diameter is 40.90 mm (DN 40), the flow velocity is 1.5 m/s. The parameters of the 7 model cases are listed in Table 1. Cases 2, 6 and 7 are designed for the mesh independence study. Cases 1 – 5 are designed for the study of inlet boundary conditions. Case 2 is the reference which is the selected mesh.

Figure 5. Average agent concentrations at the different mid-planes ( $x = u_0 \cdot t$ ) for model cases as described in Table 1. The inner pipe diameter is 40.90 mm (DN 40), the flow velocity is 1.5 m/s. Equation 1 indicates that  $C_m = 0.5 \text{ kg/m}^3$  at  $x = u_0 \cdot t$ . Cases 1 - 5 result in the same average agent concentrations (with precision  $0.00001 \text{ kg/m}^3$ ), which are displayed as overlapping symbols.

Figure 6. Comparison of the Taylor model and the CFD simulations at 1.5 m/s of flow velocity for (A) a fixed distance of 15 m with varied rinsing time, and (B) a fixed rinsing time of 10 s with varied distance.

Figure 7. Axial velocity and turbulent kinetic energy at the distance of 15 m and for a mean flow velocity of 1.5 m/s for different pipe diameters ( $Re = 26500 \sim 259000$ ).  $r / R$  is the dimensionless distance from the center of the pipe to the wall. The values of  $u_x$  and  $k$  quantify the intensity of convection in the axial direction when the radial velocity and tangential velocities are not significant in the pipe.

Figure 8. The product of displacement time and flow velocity for different pipe lengths. The marker values and error bars (too small to be seen) are from the CFD models for the simulated pipe diameters, representing the average and standard deviation of  $t_{1 \text{ or } 99} \cdot u_0$  at three flow velocities. The curves represent the values which are calculated by the power function in equation 7.

Figure 9. Agent distribution in a 1 m pipe section at different rinsing times. The inner pipe diameter is 26.64 mm (DN 25 mm), and the flow velocity is 1.5 m/s.

Figure 10. Intermediate rinse length between two cleaning agents. The intermediate rinse length equals the sum of the mixing zone of agent A, the mixing zone of agent B and an intermediate length between two mixing zones. The minimum intermediate rinse length is when the intermediate length between two mixing zones is zero.

Figure 11. Dynamic mixing length of the 77.90 mm diameter (DN 80) pipe at 1 m/s and 2 m/s.  $\Delta x$  is the relative position of the leading edge (+) and the trailing edge (–) to the mid-plane ( $x = u_0 \cdot t$ )

Figure 12. Correlation of the mixing length with the characteristic length,  $2\sqrt{K \cdot t}$ . The mixing lengths of different pipe diameters at different flow velocities are proportional to the characteristic length, which can be expressed by a first order equation with high correlation coefficient.

Figure 13. The algorithm for understanding and controlling the rinse of straight pipes based on the findings in this study. The algorithm is only valid if the flow is turbulent.

**Tables and captionss**

Table 1. Parameters for the mesh study and for the influence of turbulence intensity and turbulence length scale. The inner pipe diameter is 40.90 mm (DN 40), the flow velocity is 1.5 m/s. Case 2 is the reference case which is selected for other studies.

Case	Mesh indexes	No. of nodes in radial / axial directions	$Ti_b$ [%]	$l_b$ [% of diameter]	$y^+$	Maximum Courant number	Mean Courant number
1	Mesh 1	21 / 501	1	10	45	0.69	0.26
2	Mesh 1	21 / 501	5	10	45	0.69	0.26
3	Mesh 1	21 / 501	20	10	45	0.70	0.26
4	Mesh 1	21 / 501	5	5	45	0.69	0.26
5	Mesh 1	21 / 501	5	30	45	0.69	0.26
6	Mesh 2	29 / 751	5	10	32	1.04	0.39
7	Mesh 3	27 / 501	5	10	4	0.81	0.24

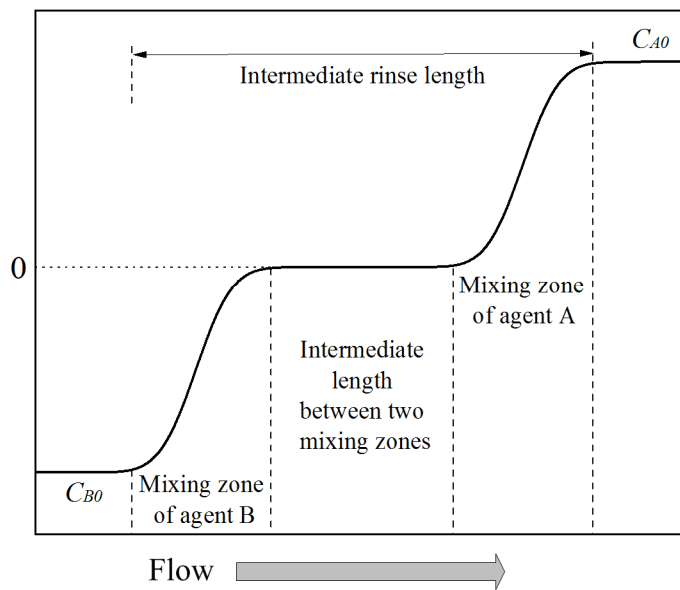
Table 2. Correlation parameters of the product of displacement time and flow velocity for different pipe lengths by the power function as equation 7. The unit of inner pipe diameter should be meter. Depending on the practical cases, the correlation parameters of other pipe lengths can also be extracted from the CFD simulation results.

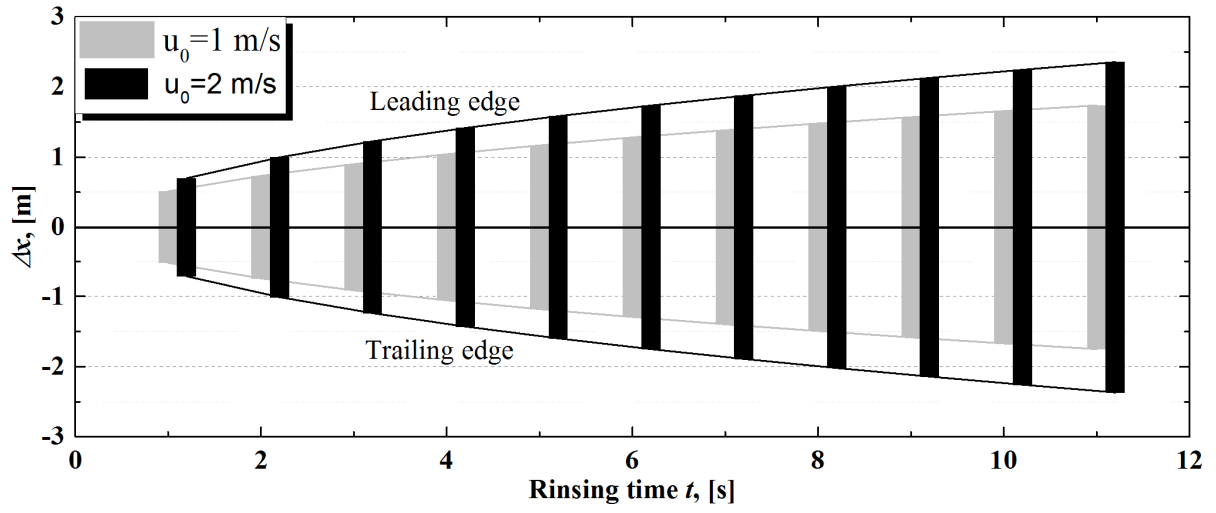
$x, [m]$	$t, [s]$	$\alpha, [m^{1-\beta}]$	$\beta$	$R^2$
2	$t_{1,plane}$	1.01	-0.121	0.998
	$t_{99,plane}$	3.83	0.107	0.963
	$t_{99,volume}$	3.03	0.0788	0.966
15	$t_{1,plane}$	11.7	-0.0456	0.989
	$t_{99,plane}$	19.1	0.0422	0.978
	$t_{99,volume}$	16.4	0.0212	0.970
24	$t_{1,plane}$	19.8	-0.0354	0.996
	$t_{99,plane}$	29.1	0.0337	0.980
	$t_{99,volume}$	25.5	0.0152	0.971

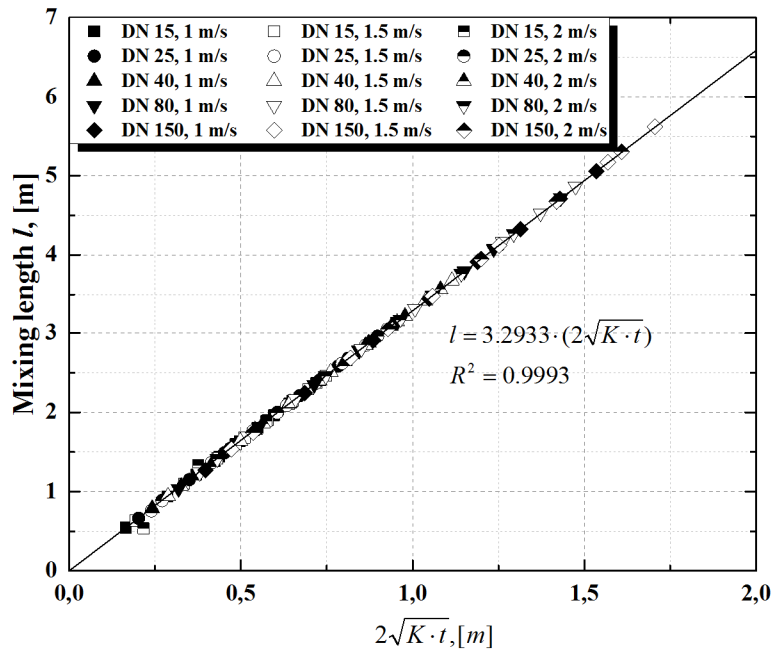


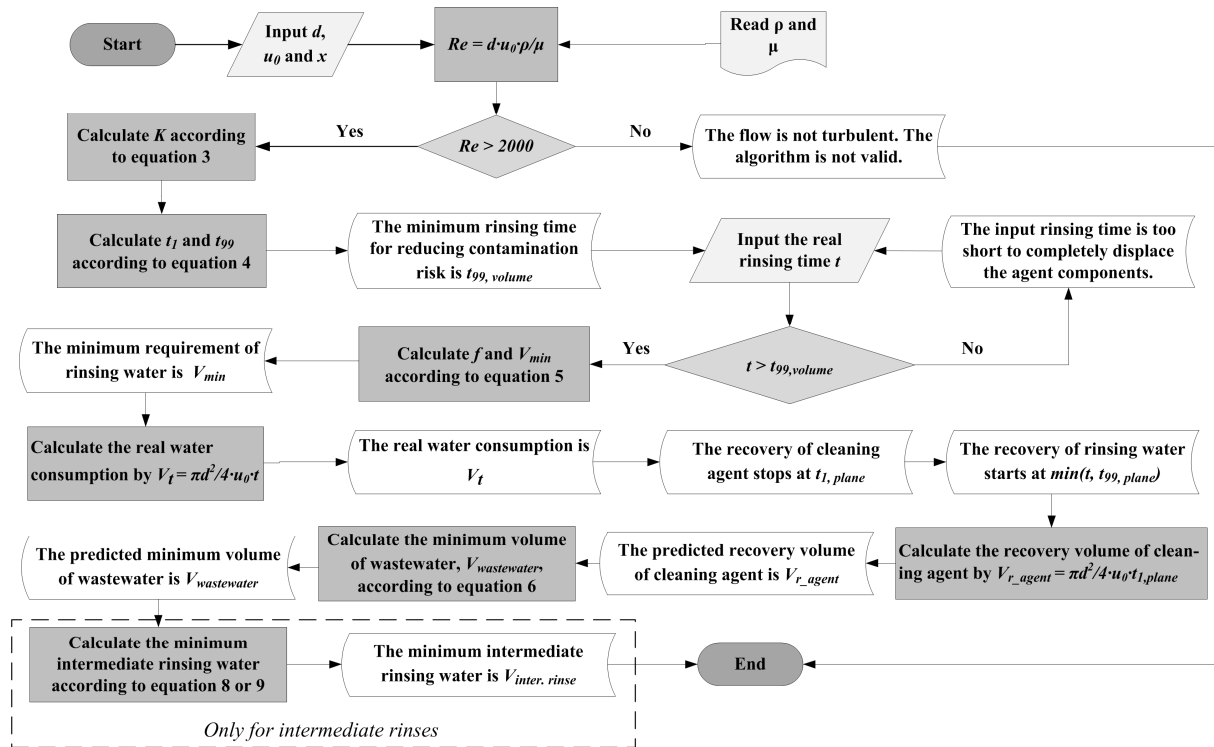
Table 3. Result summary of the case study for rinsing a 24 m straight pipe with inner diameter 100 mm. The analysis follows the algorithm depicted in Figure 15.

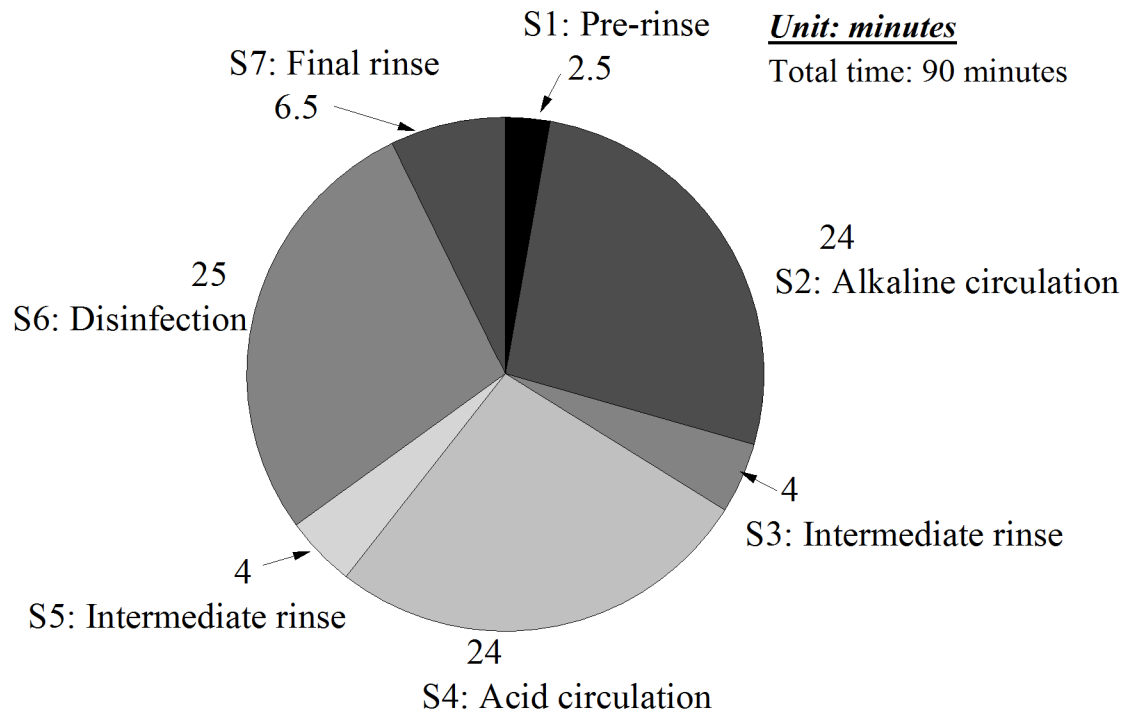
$u_0$ , [m/s]	1	1.5	2
$Re$	112035	168053	224070
Turbulence or not?	Yes	Yes	Yes
$K$ , [m <sup>2</sup> /s]	0.0316	0.0450	0.0579
$t_{1,plane}$ , [s]	21.43	14.29	10.72
$t_{99,plane}$ , [s]	31.43	20.95	15.71
$t_{99,volume}$ , [s]	26.42	17.62	13.21
$f_{plane}$	1.038	1.038	1.038
$f_{volume}$	1.154	1.154	1.154
$V_{min,plane}$ , [m <sup>3</sup> ]	0.218	0.218	0.218
$V_{min,volume}$ , [m <sup>3</sup> ]	0.196	0.196	0.196
$V_{min,plane}/V_{min,volume}$	1.112	1.112	1.112
Real rinsing time $t = 1.5 \cdot x/u_0$ , [s]	36	24	18
$t/t_{99,volume}$	1.36	1.36	1.36
Time to start the recovery of rinsing water, [s]	31.43	20.95	15.71
Real water consumption $V_t$ , [m <sup>3</sup> ]	0.283	0.283	0.283
Recovery of cleaning agent solution, [m <sup>3</sup> ]	0.168	0.168	0.168
Recovery percentage of cleaning agent solution, [%]	89.3	89.3	89.3
Minimum amount of wastewater, [m <sup>3</sup> ]	0.079	0.079	0.079
$V_{inter. rinse}$ , [m <sup>3</sup> ]	0.090	0.088	0.086
$(V_{min,volume} - V_{inter. rinse})/V_{min,volume}$	0.539	0.551	0.559

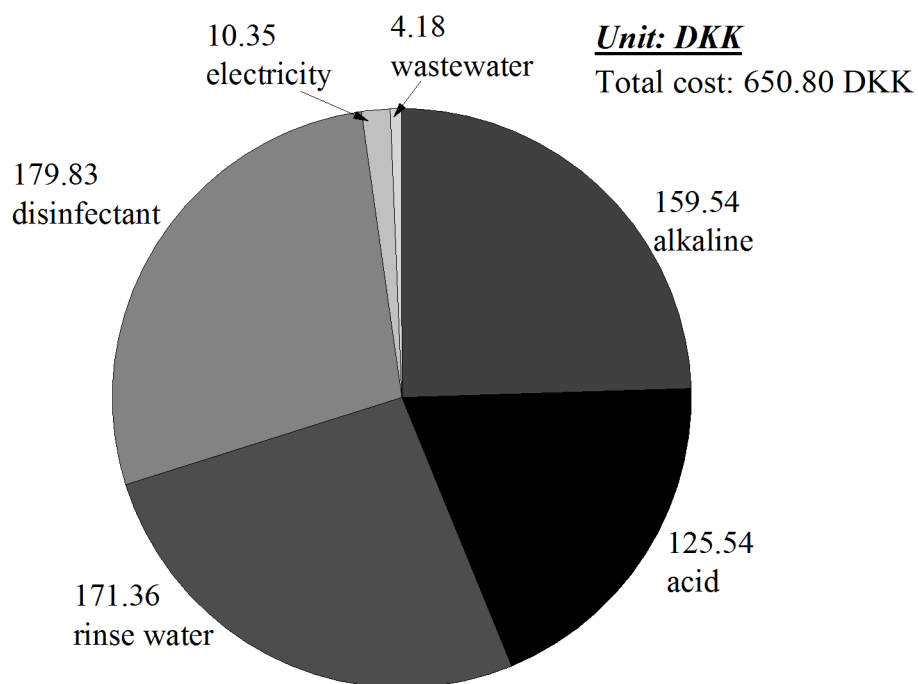


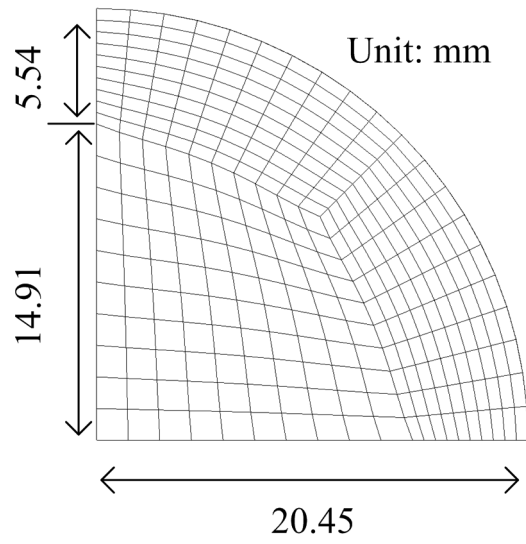






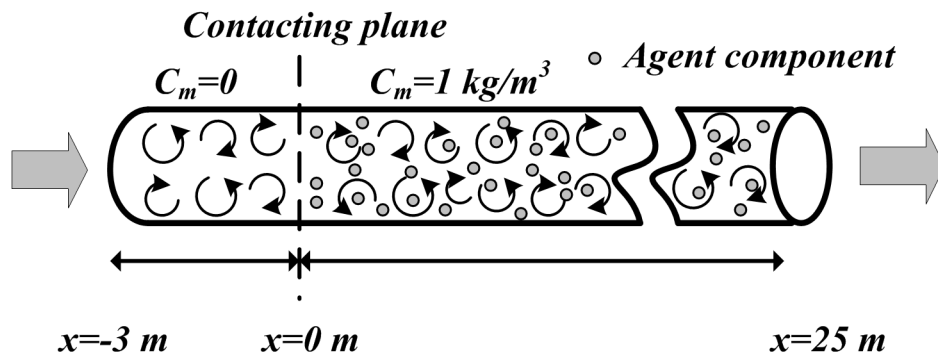






ACCEPTED MANUSCRIPT



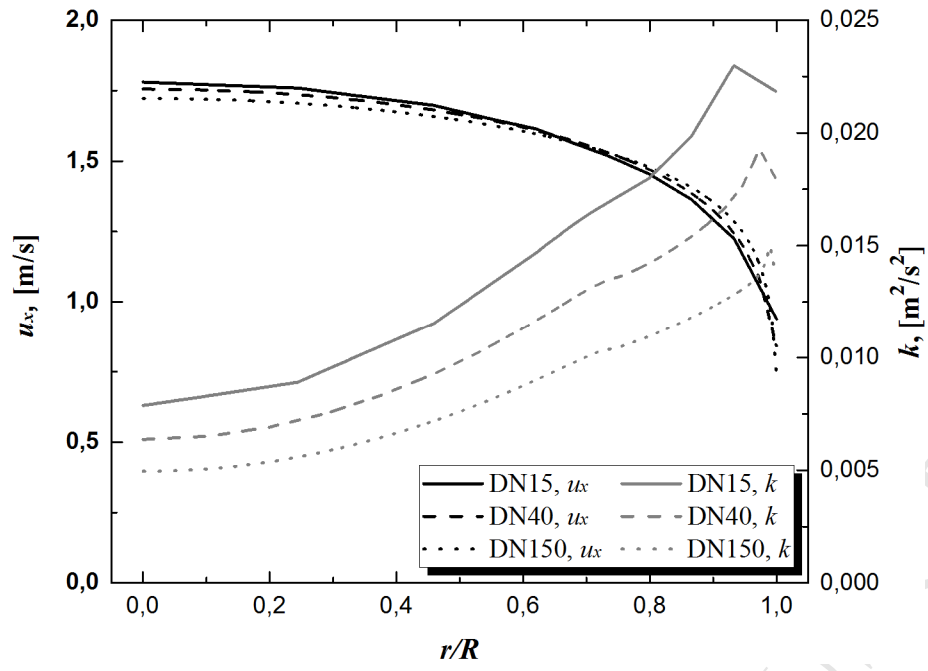


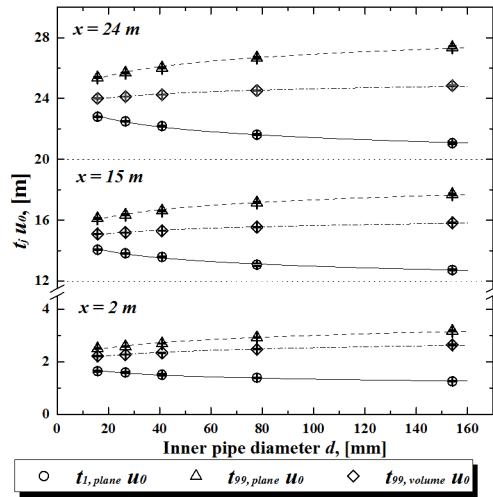


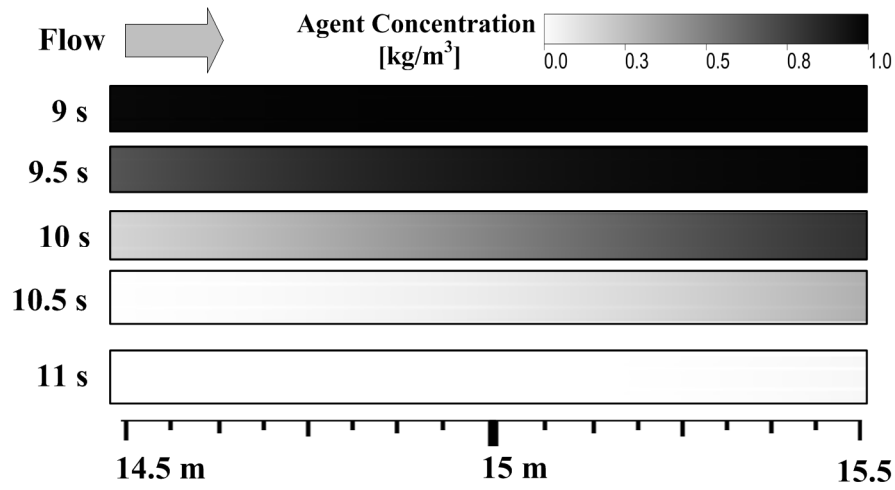














**Highlights**

- CFD simulates the axial mixing which occurs during the intermediate and final rinses during cleaning of straight pipes.
- The CFD results are in good agreement with the analytical models from literature.
- The model quantifies the minimum rinsing time, minimum water consumption and how to efficiently recover the cleaning agent and rinsing water.
- An algorithm and a case study show how to use the investigated knowledge to solve practical problems.