Model Predictive Hydrodynamic Regulation of Microflows

Leonidas G. Bleris, Jesus Garcia and Mayuresh V. Kothare

Abstract— **An application of model predictive hydrodynamic regulation of a flow stream in a microfluidic geometry is provided in this paper. Using bit-accurate emulations we mimic the optimization operations, carried out in an embedded 32-bit microcontroller. Additionally, finite element method simulations are utilized to solve the coupled partial differential equation problem that describes the dynamics of the examined system. A combination of these simulations and hardware emulations allows us to apply real-time predictive control to the microflows by adjusting the inlet streams at the macroscopic level.**

I. Introduction

Applying control in a microchemical system may include efficient mixing of different laminar streams, manipulating microflows and adjusting the temperature distribution. From a control perspective we face the following challenges. Firstly, the development of an efficient controller capable of handling the high dimensional models of these Systems-on-a-Chip (SoC) and secondly reducing its complexity so that it can be implemented on a chip and subsequently embedded with the rest of the system. While the control of fluid flows has been an active research area, there is very little work in literature on the dynamics and control of microflows in these highly functional and versatile SoC. Given the ability to accurately measure velocity profiles within microchannels and concentration at the outlets, active manipulation of microflows can be achieved [1] by applying control both at the macroscopic level or within the microchannels. The simplest approach is to apply control using specific inlets and outlets at the macroscopic level. A resulting drawback is the inability to apply distributed control from the macroscopic level. Within the microchannels, control can be applied using different kinds of external fields. The application of electrostatic fields, electromagnetic forces, sound and capillary effects [1] has been reported in literature.

II. Real-time Model Predictive Control

Model Predictive Control (MPC) originated in the chemical process industries. The main advantages of MPC are the ability to handle constraints and its applicability to multivariable nonlinear processes. Because of the computational requirements of the optimizations associated with MPC, it has primarily been applied to plants in the process industry, with slow dynamics. Furthermore, existing implementations of MPC typically perform numerical calculations using workstations in 64-bit Floating Point (FP) arithmetic, which is too expensive, power demanding and large in size. Therefore the application of real-time embedded model predictive control for microscale devices presents new technological challenges.

To this end, some initial approaches have been recently reported in literature. A work that addresses the issue of finding the programming procedure that results in the fastest implementation of the core calculations of model predictive control algorithms, amenable to parallel processing on a real-time multiprocessing system is provided in [2]. The combination of the new technology of Field-Programmable Analog Arrays (FPAAs) with the more commonly used technology of Field-Programmable Gate Arrays (FPGAs) was proposed in [3], for the development of dynamically reconfigurable analog/digital hardware capable of handling MPC computation requirements. Since the MPC algorithm is iterative, the feedback scheduler may also abort a task prematurely to avoid excessive input-output latency. A feedback scheduling strategy for multiple MPCs is proposed in [4], where the scheduler allocates CPU time to the tasks according to the current values of the cost functions. Recently a multi-parametric programming method was proposed [5], [6] to solve off-line the quadratic optimization problem associated with MPC. The constrained quadratic optimization is shown to be piecewise affine, using partitions of the state space determined by the constraints. The feedback laws are pre-computed and online calculations consist of a table-lookup in memory and an affine transformation. However, for an input constrained problem, increasing the number of controlled variables (thus the number of constraints), yields prohibitive memory requirements for multivariable constrained systems with fast dynamics.

Alternatively, we have proposed [7], [8] a parametric emulation based methodology for reducing the precision of a microprocessor to the minimum while maintaining optimal control performance. By reducing the precision we are increasing the optimization speed while reducing the power consumption and the overall chip area. Taking advantage of the low precision, a Logarithmic Number System (LNS) based microprocessor architecture is used [9], providing further energy and computational cost savings.

An application of model predictive hydrodynamic regulation of a flow stream in a microfluidic geometry is provided in this paper. We utilize computational tools to simulate the microfluidic dynamics and bit-accurate hardware emulations

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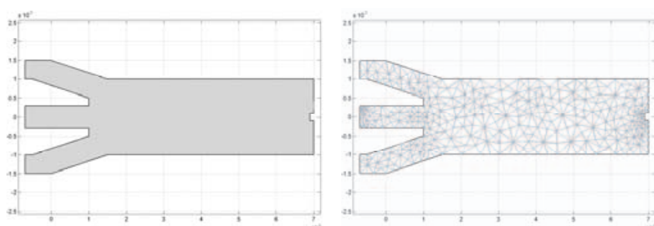
to mimic the MPC chip operations. More specifically, using a Finite Element Method (FEM) tool we simulate a complex geometry under MATLAB environment where we additionally emulate the microcontroller arithmetic operations using C++ code. For this work 32-bit word sizes are used for the arithmetic operations. Emulation results [8] indicate that the minimum sampling time of this microcontroller is sufficiently fast to capture the dynamics of the examined system.

This paper is organized as follows. Section III contains the problem formulation; that is the microfluidic geometry examined, the governing equations and some initial simulations. In Section IV, we provide the main theoretical aspects of model predictive control, details on the optimization approach and the creation model used by MPC. Two case studies are examined in Section V and we provide the simulation-emulation results. We conclude the paper with remarks on our research results and an analysis of issues that are currently under investigation.

III. Problem Formulation

Consider the microfluidic geometry of Figure 1. There are three inlets (left side) and two outlets (right side). The middle inlet from the left side allows the introduction of chemicals in the microgeometry. The outer left inlets (top and bottom) are used in order to steer the chemicals to one of the two outlets; this is accomplished by adjusting the inlet velocities at the macroscopic level.

There are numerous potential control applications for this microfluidic "switch". By adjusting the outer left inlet streams we can direct the chemicals inserted by the middle inlet to the desired outlet for further processing. For instance, the two outlets of the geometry can be connected to two mass spectrometers (instruments which can measure the masses and relative concentrations of atoms and molecules). Another application can be found in microchemical systems [10]; the two outlets can be connected to different size chambers or chambers with different catalysts.



(a) (b)

Fig. 1. Microfluidic system (a) geometry and (b) finite element mesh.

In order to build this geometry we utilize FEMLAB [11], an interactive environment for modeling and simulating scientific and engineering problems based on Partial Differential Equations (PDEs). For the numerical integration of the coupled PDEs that describe the dynamics of our microfluidic system, we use standard MATLAB functions. Furthermore, we use the ability to export spatiotemporal snapshots of the concentration and the velocity profiles of the simulated system, thereby allowing a rigorous analysis of the dynamics and most importantly allowing the integration of the emulated MPC under MATLAB environment.

A. Governing Equations

In order to study the flow streams in the examined geometry we define momentum balances in spatial directions, and combine these balances with the continuity equation. That is, we form a momentum balance for each of the components of the velocity vector **v** in the different spatial dimensions (in the x, y directions, neglecting the z dependence) to obtain the Navier-Stokes equations:

$$\rho\frac{\partial \mathbf{v}}{\partial t} - \nabla\cdot\eta(\nabla\mathbf{v} + (\nabla\mathbf{v})^T) + \rho(\mathbf{v}\cdot\nabla)\mathbf{v} + \nabla p = 0 \quad (1)$$

$$\nabla\cdot(\rho\mathbf{v}) = 0 \quad (2)$$

where ρ is the density and η the viscosity. To solve the above coupled problem we need to define the boundary conditions. For the Navier-Stokes equations we define the boundary conditions to be no-slip at the walls; we also assume fully developed laminar flow at the outlet (the velocity components tangential to the boundary are zero). Note that the Reynolds number is well inside the laminar flow region (common in microchannel fluid flows). Thus we can get a numerical solution of the full momentum balance and continuity equations.

In order to simulate the dynamic behavior of the chemicals inserted in the middle inlet we assume Fickian diffusion of dilute species. To describe the diffusive transport in the microchannel we use the convection-diffusion equation given by:

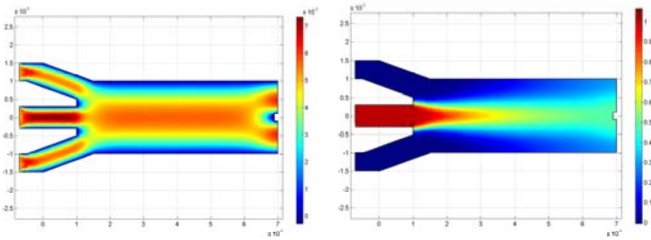
$$\frac{\partial \mathbf{C}}{\partial t} - \nabla(-D\nabla\mathbf{C} + \mathbf{C}\mathbf{v}) = 0 \quad (3)$$

where D denotes the diffusion coefficient and **C** is the concentration of the inserted chemical species.

We assume that the density ρ and the viscosity η remain constant. The density of the fluid ρ is set at 1000kg/m^3, and the viscosity η at 0.001 kg/m·. We also define the diffusion coefficient $D = 1.26\times10^{-7}m^2/sec$. For boundary conditions we define an initial concentration $\mathbf{C}_0$ at the middle inlet, the walls are defined as non-permeable, and at the outlet of the microchannel the convective transport is assumed to be much larger than the diffusive transport (sometimes called the Danckwerts boundary condition).

B. Finite Element Method Simulations

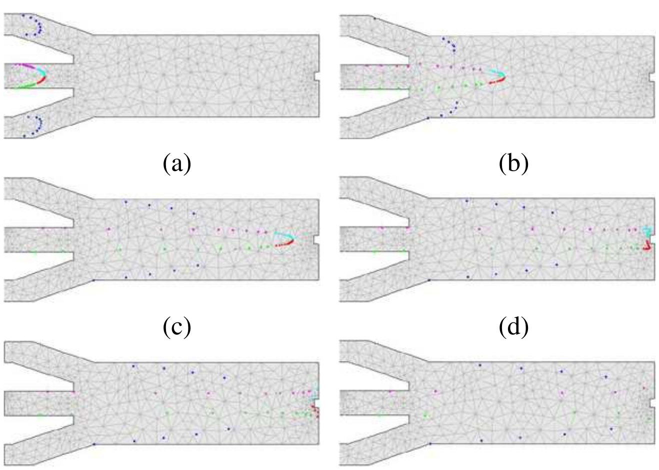
We provide initial velocity of v=5mm/sec at all the inlets. For this study we use two manipulated variables; the velocities of the top and bottom inlets. These velocities correspond to the maximum velocity of the applied parabolic (see Figure 3(a)) velocity profile. The solution for the velocity profile is given in Figure 2(a), while the concentration distribution profile in Figure 2(b).



(a) (b)

Fig. 2. (a) Fluid flow velocity profile for inlet velocities at 5mm/sec and (b) concentration profile.

Taking advantage of the numerical capabilities of FEMLAB we track flow streams that are inserted in the geometry, and we examine their spatiotemporal behavior. From Figure 3 it is illustrated that as expected under equal inlet velocities the particles inserted into the middle channel are separated symmetrically at the outlet. The subplots correspond to different time instances within 1sec from the time that the particles enter the micro-geometry. The control objective is to adjust appropriately the inlet velocities at the control inlets in order to obtain a desirable distribution of the chemicals (inserted from the middle inlet) at the outlet.



(a) (b) (c) (d) (e) (f)

Fig. 3. Spatiotemporal distribution of particles in the geometry.

IV. Model Predictive Control

Model predictive control is also known as receding horizon control or moving horizon control. Controllers belonging to the MPC family are generally characterized by the following steps:

Initially the future outputs are calculated at each sample interval over a predetermined horizon N, the prediction horizon, using the process model. These outputs $y(t+k|t)$ for $k = 1...N$ depend up to the time t on the past inputs and on the future signals $u(t+k|t)$, $k = 0...N-1$ which are those to be sent to the system.

The next step is to calculate the set of future control moves by optimizing a determined criterion in order to keep the process as close as possible to a predefined reference trajectory. This criterion is usually a quadratic function of the difference between the predicted output signal and the reference trajectory. In some cases the control moves $u(t+k|t)$ are included in the objective function in order to minimize the control effort:

$$J_P(k) = \sum_{k=0}^{P} \{[y(t+k|t) - y_{ref}]^2 + Ru(t+k|t)^2\} \quad (4)$$

$$|u(t+k|t)| \leq b \quad , \quad k \geq 0 \quad (5)$$

where $y(t+k|t)$ are the predicted outputs, y_{ref} is the desired set reference output, $u(t+k|t)$ the control sequence and R is the weighting on the control moves, a design parameter. This system is subject to input constraints given by the vector b.

Finally, the first control move $u(t|t)$ is sent to the system while the rest are rejected. This is because at the next sampling instant the output $y(t+1)$ is measured by the system and the procedure is repeated with the new values so that we get an updated control sequence.

The schematic of the overall system is given in Figure 4.

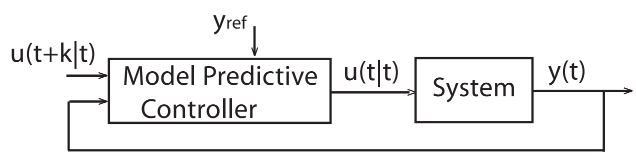


Fig. 4. Block diagram of MPC.

A. *Impulse Response Model*

There are many models used in different formulations [12] of MPC. These include step response models, impulse response models, transfer function models and state space models. In this paper we use the geometry of Figure 5, we define the Navier-Stokes and the convection-diffusion equations on the microchannel domain, we add the boundary conditions and we use impulse response model for the predictive control problem formulation. Notice that the geometry from which we create the impulse response model is almost identical to Figure 1. The only difference is that we model the evolution of the streams in the microchannels up to 1mm distance from the two outlets (at 6mm). This is done in order to minimize the computational costs associated with the FEM simulations.

In order to create the impulse response model we apply an impulse change of 5mm/sec magnitude, from the steady state velocities of Figure 2, to each of the inlets separately. We measure the velocities and concentrations at the locations close to the outlets, indicated with the symbol "x" in Figure 5.

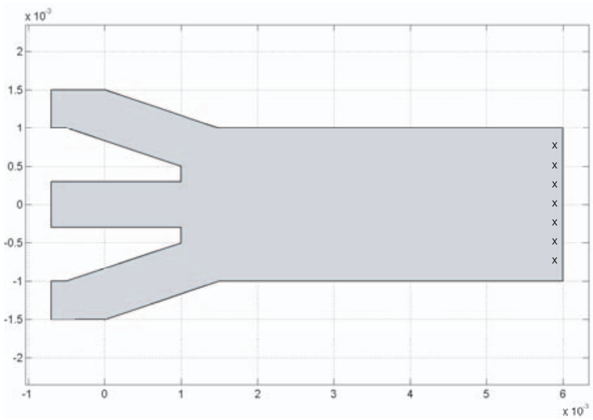


Fig. 5. Geometry used to create the MPC model.

B. Optimization

Quadratic programming (QP) is an algorithm that allows solving this optimization problem, and obtaining the exact solution in a bounded number of steps [13]. Note that the solution of QP is exact as long as operations are carried out with sufficient precision; with reduced precision this advantage disappears. The quadratic problem can be defined as:

$$\begin{aligned} \underset{\mathbf{x}}{\text{minimize}} \quad & q(\mathbf{x}) \triangleq \frac{1}{2}\mathbf{x}^T\mathbf{G}\mathbf{x} + \mathbf{g}^T\mathbf{x} \\ \text{subject to} \quad & \mathbf{a_i}^T\mathbf{x} = b_i, \quad i \in E \\ & \mathbf{a_i}^T\mathbf{x} \geq b_i, \quad i \in I, \end{aligned} \tag{6}$$

where $\mathbf{G}$ is the Hessian matrix and can be defined as symmetric without loss of generality. The set E defines the equality constraints, and the set I represents the inequality constraints. If the problem (6) has a solution, and $\mathbf{G}$ is positive definite, the solution $\mathbf{x}^*$ is unique and represents a global minimum.

Following the description of [13], the problem of (6) can be solved using the active set algorithm. An active set $\mathcal{A}$ comprises of those constraints that are regarded as active; active constraints are considered the equality constraints, and the inactive ones are ignored. In iteration k, a feasible solution $\mathbf{x}^{(k)}$ satisfies $\mathbf{a}_i^T\mathbf{x}^{(k)} = b_i$, $i \in \mathcal{A}$, while $\mathbf{a}_i^T\mathbf{x}^{(k)} > b_i$, $i \notin \mathcal{A}$ (except in degenerate cases). In each iteration, a solution to the equality constrained problem (i.e., problem (6) where $I = \{\emptyset\}$) defined using only the constraints in $\mathcal{A}$ is sought. Moreover it is suggested in [13] that the origin can be shifted to $\mathbf{x}^{(k)}$, in order to obtain the incremental problem:

$$\begin{aligned} \underset{\delta}{\text{minimize}} \quad & \frac{1}{2}\delta^T\mathbf{G}\delta + \delta^T\mathbf{g}^{(k)} \\ \text{subject to} \quad & \mathbf{a_i}^T\delta = \mathbf{0}, \quad i \in \mathcal{A}, \end{aligned} \tag{7}$$

where $\mathbf{g}^{(k)} = \nabla q(\mathbf{x}^{(k)}) = \mathbf{G}\mathbf{x}^{(k)} + \mathbf{g}$ is obtained for $q(\mathbf{x})$ defined in (6). The QP algorithm [13] can be formally enunciated as:

1) Given $\mathbf{x}^{(1)}$ and $\mathcal{A}$, set $k = 1$.
2) If $\delta = \mathbf{0}$ does not solve (7), go to 4.
3) Compute Lagrange multipliers $\lambda^{(k)}$ and solve

$$\min_{i \in \mathcal{A} \cap I} \lambda_i^{(k)}; \tag{8}$$

if the solution to (8) $\lambda_q^{(k)} \geq 0$, terminate with $\mathbf{x}^* = \mathbf{x}^{(k)}$, else remove q from $\mathcal{A}$.
4) Solve equation (7).
5) Find $\alpha^{(k)}$ as:

$$\alpha^{(k)} = \min \left(1, \quad \min_{\substack{i \,:\, i \notin \mathcal{A}, \\ \mathbf{a}_i^T\delta^{(k)} < 0}} \frac{b_i - \mathbf{a}_i^T\mathbf{x}^{(k)}}{\mathbf{a}_i^T\delta^{(k)}} \right) \tag{9}$$

and set $\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha^{(k)}\delta^{(k)}$.
6) If $\alpha^{(k)} < 1$, add its index p (from (9)) to $\mathcal{A}$.
7) Set $k = k + 1$ and go to step 2.

To solve the QP algorithm, the solution $\mathbf{x}^{(k)}$ to an equality-constrained problem (like (7)), and its associated Lagrange multipliers $\delta^{(k)}$ need to be computed. The solution to an only equality-constrained quadratic problem (i.e., $I = \{\emptyset\}$ in (6)), is analytic. Let the equality constraints be defined by

$$\mathbf{A}^T\mathbf{x} = \mathbf{b}, \tag{10}$$

where $\mathbf{A}^T$ is formed by columns $\mathbf{a}_i^T$, $i \in E$. Using QR factorization, e.g. using Householder transformations, find $\mathbf{Y}$ and $\mathbf{Z}$ such that:

$$\mathbf{A} \underset{QR}{=} \begin{bmatrix} \mathbf{Q}_1 & \mathbf{Q}_2 \end{bmatrix} \begin{bmatrix} \mathbf{R} \\ \mathbf{0} \end{bmatrix} \left\{ \begin{array}{lcl} \mathbf{Y} & = & \mathbf{Q}_1\mathbf{R}^{-T} = \mathbf{A}^{+T} \\ \mathbf{Z} & = & \mathbf{Q}_2 \end{array} \right. \tag{11}$$

The explicit solution can be obtained as:

$$\mathbf{x}^* = \mathbf{Y}\mathbf{b} - \mathbf{Z}(\mathbf{Z}^T\mathbf{G}\mathbf{Z})^{-1}\mathbf{Z}^T(\mathbf{g} + \mathbf{G}\mathbf{Y}\mathbf{b}), \tag{12}$$

where $\mathbf{G}$ and $\mathbf{g}$ are those defined in (6). The associated Lagrange multipliers can be obtained as:

$$\begin{aligned} \delta^* = (\mathbf{Y} - \mathbf{Y}\mathbf{G}\mathbf{Z}(\mathbf{Z}^T\mathbf{G}\mathbf{Z})^{-1}\mathbf{Z}^T)\mathbf{g} + \\ \mathbf{Y}^T(\mathbf{G} - \mathbf{G}\mathbf{Z}(\mathbf{Z}^T\mathbf{G}\mathbf{Z})^{-1}\mathbf{Z}^T\mathbf{G})\mathbf{Y}\mathbf{b} \end{aligned} \tag{13}$$

C. Hardware Emulation of MPC

In addition to the FEM simulations used that represent the examined system we emulate the predictive controller. The microcontroller arithmetic operations (QP optimization) are coded using C++ code and we obtain bit-accurate results of the operations. A library of arithmetic operations defined for each particular hardware architecture is used. These operations are parameterized, allowing the simulation of the desired precision. For this work a 32bit processor is used. Overloading the standard operators in C++, the same code can be used to run using native floating point, or our emulated hardware.

V. Emulation-Simulation Results

In this section we provide the results of the application of model predictive control for two hydrodynamic regulation problems in the proposed geometry. The real-time behavior of the controller is investigated with the parallel use of emulations and FEM simulations.

A. Hydrodynamic Regulation

The control objective firstly, is to appropriately adjust the inlet streams in order to drive the chemicals inserted into the middle left inlet to the bottom right outlet. The inlet streams enter the geometry with initial velocity of 5mm/sec. The control variables are constrained at a lower bound of 5mm/sec and an upper bound of 50mm/sec. We measure the velocities and concentrations at the seven assigned locations close to the outlets (Figure 5). The optimal performance for MPC is achieved using R=0.005 and control horizon of 6 with prediction horizon of 10. The solution for the velocity profile after 40 seconds, with sampling every 1sec, is given in Figure 6. The concentration distribution profile is given in Figure 7.

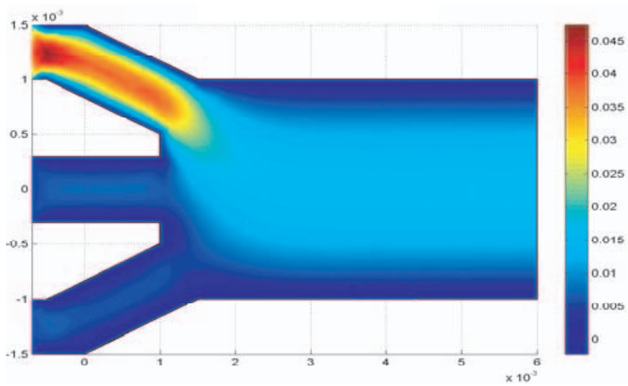


Fig. 6. Steady state velocity profile.

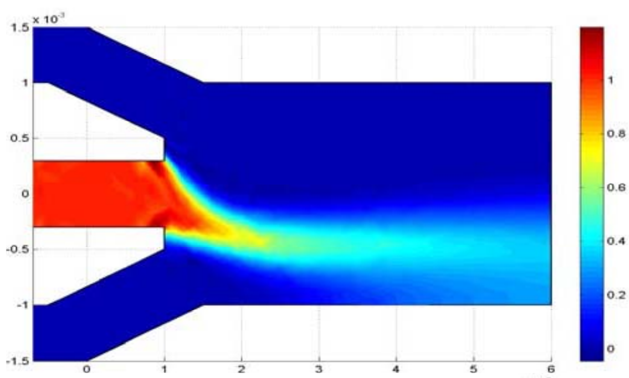


Fig. 7. Steady state concentration profile.

Additionally we track the stream of chemicals that are inserted in the microfluidic geometry and we examine their spatiotemporal behavior. As illustrated in Figure 8, the model predictive controller steers the chemical inserted from the middle inlet to the bottom outlet, thus meeting the control objective.

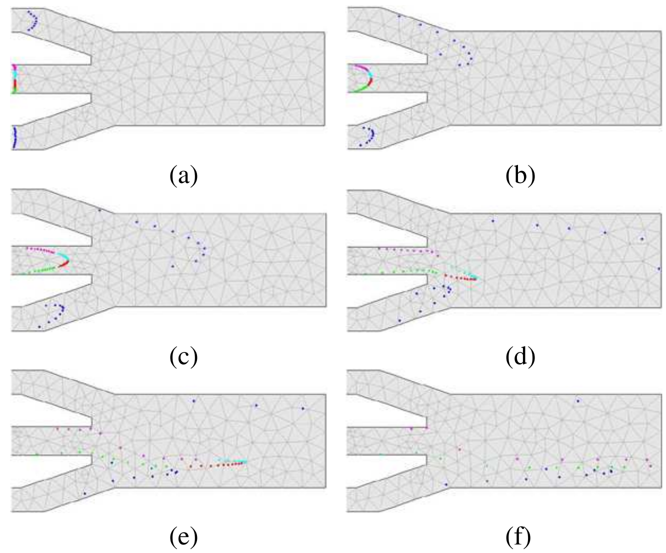


Fig. 8. Spatiotemporal distribution of inserted particles at the 40^{th} sec.

B. Switching of the Control Objective

In this second study, we want to control the stream from the middle inlet in order to alternate between the two outlets. More specifically we initially want the chemicals to exit the system from the bottom outlet and at 30 seconds we switch the objective, requiring that they exit from the outlet located at the top. We use again R=0.005 for the weight on the control moves and control horizon of 6 with prediction horizon of 10. The concentration profiles at different time instances (from the top: 5, 10, 15, 20, 25, 30^{th} second) are given in Figure 9. We then change the control objective and in Figure 10 we illustrate the concentration profiles after the switch (from the top: 35, 40, 45, 50, 55, 60^{th} second).

VI. Concluding Remarks

The application of MPC for hydrodynamic regulation of microflows has been examined in this paper. The simulation and emulation experiments that were conducted, illustrate that MPC provides an optimal sensing-control-actuation performance that cannot be achieved with simple control schemes. By reducing the precision of the operations coupled with the use of logarithmic number system arithmetic microprocessor, we can achieve sampling rates as low as 0.023sec [8]. Current work includes the real-time implementation of the proposed MPC algorithms on a high-performance 32-bit general purpose processor, and a Lyapunov based stability analysis of our proposed embedded model predictive controllers.

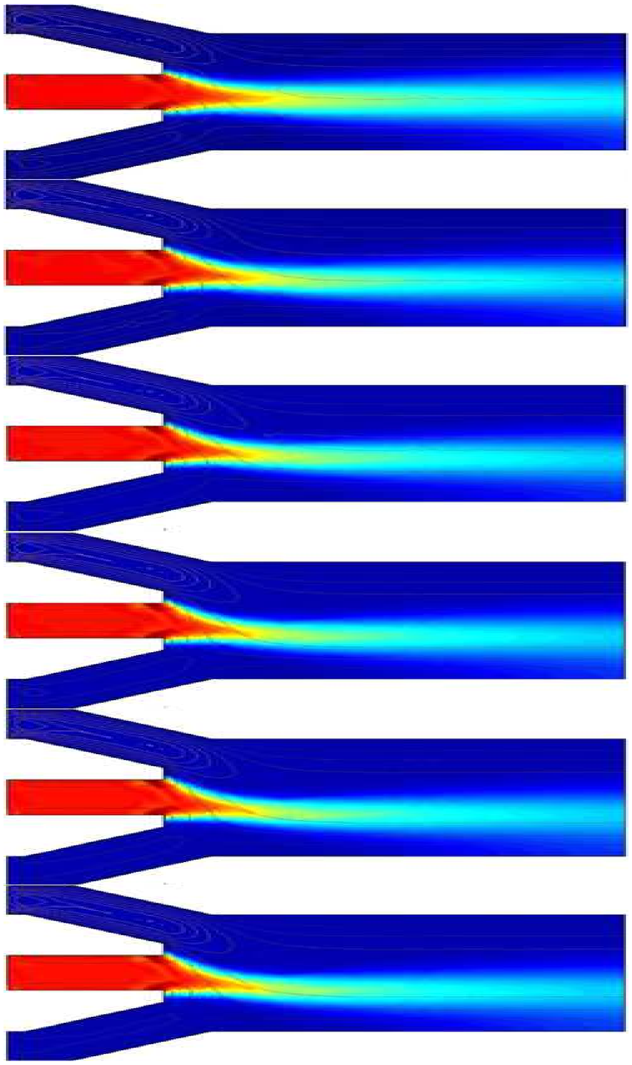


Fig. 9. Concentration profiles at consecutive time instances before switching the control objective.

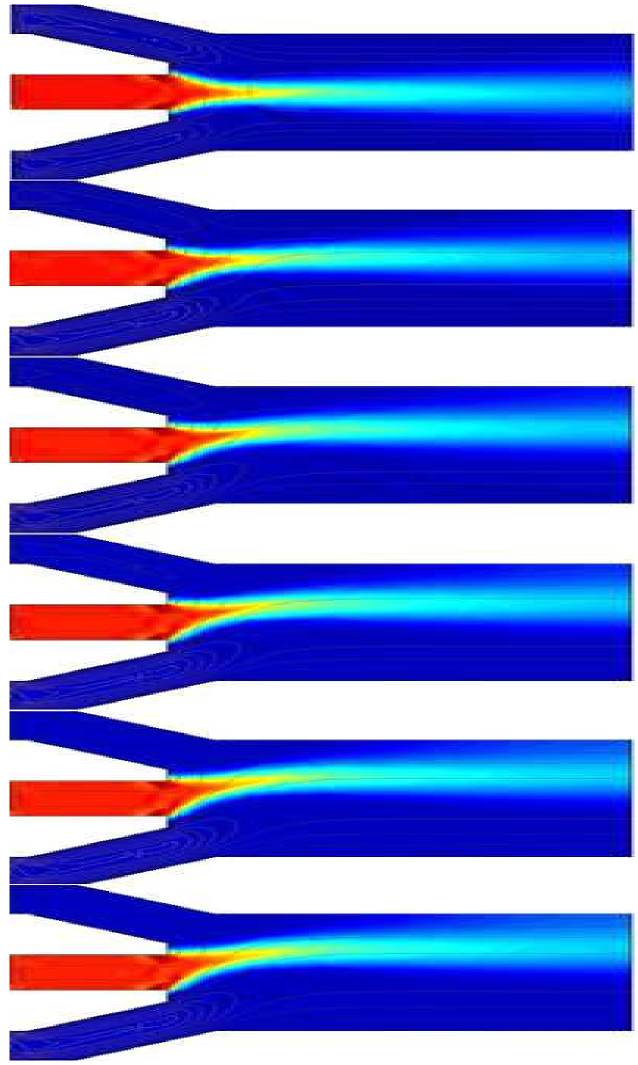


Fig. 10. Concentration profiles at consecutive time instances after switching the control objective.

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