An adjoint-based temperature boundary optimal control approach for turbulent buoyancy-driven flows

L Chirco¹, V Giovacchini¹ and S Manservisi¹

¹ Department of Industrial Engineering DIN
Laboratory of Montecuccolino
University of Bologna
Via dei Colli 16, Bologna 40136 (BO), Italy
E-mail: valentin.giovacchini2@unibo.it

Abstract. This paper deals with the adjoint optimal control for turbulent buoyancy-driven flows. The aim of this optimal control problem is to obtain a desired velocity profile and enhance the turbulence intensity in a well defined region by controlling the fluid temperature on domain boundaries and consequently the buoyancy forces. The fluid is assumed to be incompressible within the Boussinesq approximation, while turbulence is considered by coupling the Wilcox k-ω model with the Reynolds Averaged energy and Navier Stokes equations. The state, adjoint and control equations are derived by employing the Lagrangian multipliers method. The optimality system is solved with a finite elements code where a steepest descent algorithm has been implemented in order to find the optimal boundary control parameter. Numerical results are reported to show the robustness of the method in solving strongly-coupled optimality systems with a large number of unknowns.

1. Introduction

The optimal control of the energy and Navier-Stokes equations arouses interest in a variety of engineering fields. Natural convection systems optimal design is crucial in many contexts, ranging from thermal-hydraulics of lead-cooled fast reactors where cooling is guaranteed by natural convection, to semiconductor production processes where buoyancy forces control the crystal growth.

Optimal control tools are nowadays available in CFD commercial software. The interested reader for real world and commercial tools can find, for example, details in ANSYS FLUENT [1] and references cited therein. In past years, considerable progresses have been made in mathematical analysis and computations of optimal control for natural convection flows. Optimal control problems for the thermally coupled Navier-Stokes equations within the Boussinesq assumptions have been considered in several works focusing on the stationary Neumann or Dirichlet boundary control [2, 3, 4, 5]. Distributed control problems have been approached in order to find the optimal heat source or force in case of electrically conductive fluids [6]. Some attempts have been made for controlling non-stationary flows solving a time-dependent optimal control problem [7, 8]. However, very few cases of optimal control problems for buoyancy-driven turbulent flows have been studied. On the other hand, turbulent flows
adjoint control has been studied in several past works [9, 10, 11], but the flow temperature dependence has never been considered.

In heat transfer applications turbulent flows usually occur, therefore it is crucial to study an adjoint optimal control formulation for non-isothermal turbulent flows. It is useful for many industrial applications to be able to control turbulence either to reduce it or, in some cases, to increase it, by acting on velocity or temperature fields.

In this article we treat optimal control problems for the stationary Reynolds-Averaged Boussinesq equations closed with a $k$-$\omega$ model in a square cavity. We consider an adjoint boundary control problem for steady incompressible thermally convected turbulent flows, in order to find an optimal boundary temperature that minimizes a functional computed for different objectives. In the first case we aim at matching the velocity field in a region of the cavity with a desired profile. In the second case, we seek to enhance the turbulence inside the cavity. In both cases, the goals are accomplished by changing the temperature in a cavity wall. We first derive, by applying the Lagrangian multipliers method, the optimality system which consists of the state, adjoint and control equations and then present numerical results by using a steepest descent algorithm for the search of the local minimum of the functional.

2. Mathematical model

In this section we introduce the mathematical model describing our optimal control problem. We denote with $L^2(\Omega)$ the space of square integrable functions and with $H^s(\Omega)$ the standard Sobolev space with norm $\|\cdot\|_s$. We denote with $H^1(\Gamma)$ the trace space for the functions in $H^1(\Omega)$ and its dual with $H^{-1}(\Gamma)$. Given any subset $\Gamma_s \subset \Gamma$, $H^1(\Omega)$ is the subspace of $H^1(\Omega)$ containing functions with vanishing trace on $\Gamma_s$. For more details on these spaces, the reader can consult [12].

2.1. Governing equation of a buoyancy-driven turbulent flow

We consider the Reynolds-Averaged heat and Navier-Stokes equations for a turbulent fluid flowing inside a heated cavity. The Reynolds stress tensor and the turbulent heat flux are modeled with mean velocity and temperature gradient components and two turbulent diffusion coefficients, the eddy kinematic viscosity $\nu_t$ and the eddy thermal diffusivity $\alpha_t$. The $k$-$\omega$ two-equations model guarantees the closure of the system and an accurate evaluation of the eddy kinematic viscosity $\nu_t$ as the ratio between the turbulent kinetic energy $k$ and its specific dissipation rate $\omega$. The eddy thermal diffusivity $\alpha_t$ is supposed proportional to $\nu_t$ through turbulent Prandtl number $Pr_t$, according to the similarity assumption between velocity and temperature fields. Typically $Pr_t$ ranges from 0.7 to 0.9 depending on the fluid Prandtl number $Pr$. In a first approximation we consider $Pr_t$ constant and equal to its average value assumed for most of fluids, namely we set $Pr_t = 0.85$. We model the flow as incompressible according to the Oberbeck-Boussinesq approximation, that neglects fluid density variations risen by the temperature in the advective term. Density temperature dependence cannot be neglect in the buoyancy force and a linear dependence is taken into account through fluid coefficient of expansion $\beta$. The governing equations for a buoyancy-driven turbulent flow can be written as follows [13]

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

\[
(\mathbf{u} \cdot \nabla) \mathbf{u} + \nabla p - \nabla \cdot [(\nu + \nu_t) \mathbf{S}(\mathbf{u})] = \mathbf{f}_b, \quad (2)
\]

\[
(\mathbf{u} \cdot \nabla) k - \nabla \cdot [(\nu + \sigma_k \nu_t) \nabla k] = P_k - \varepsilon_k + P_{k,b}, \quad (3)
\]

\[
(\mathbf{u} \cdot \nabla) \omega - \nabla \cdot [(\nu + \sigma_\omega \nu_t) \nabla \omega] = P_\omega - \varepsilon_\omega + P_{\omega,b}, \quad (4)
\]

\[
(\mathbf{u} \cdot \nabla) T - \nabla \cdot [(\alpha + \alpha_t) \nabla T] = 0, \quad (5)
\]

2
\[ \nu_t = \frac{k}{\omega}, \quad \alpha_t = \frac{\nu_t}{Pr_t}, \]  

(6)

where \( S(\mathbf{u}) \) is the strain rate tensor, \( f_b \) is the specific buoyancy force, \( P_k, P_\omega, \varepsilon_k \) and \( \varepsilon_\omega \) are respectively the production and dissipation terms of Reynolds stress for \( k \) and \( \omega \), while \( P_{k,b} \) and \( P_{\omega,b} \) are source terms depending on the interaction between gravity and turbulent heat flux components

\[
S(\mathbf{u}) = \nabla \mathbf{u} + (\nabla \mathbf{u})^T, \quad \varepsilon_k = \beta_k k \omega, \quad P_k = \frac{\nu_t}{2} S(\mathbf{u}) : S(\mathbf{u}), \quad P_{k,b} = \beta \alpha t \mathbf{g} \cdot \nabla T, \\
f_b = \beta (T - T_{ref}) \mathbf{g}, \quad \varepsilon_\omega = \beta_\omega \omega^2, \quad P_\omega = \frac{c_\omega}{2} S(\mathbf{u}) : S(\mathbf{u}), \quad P_{\omega,b} = \frac{\beta}{Pr_t} \mathbf{g} \cdot \nabla T,
\]

where : denotes the double dot product of tensors, i.e. \( S(\mathbf{u}) : S(\mathbf{u}) = \sum_i \sum_j S_{ij}(\mathbf{u}) S_{ij}(\mathbf{u}) \). The coefficients depend on the chosen model. Wilcox model requires \( c_\omega = 0.52, \beta_k = 0.09 \) and \( \beta_\omega = 0.36 \). In order to complete the Reynolds Averaged energy and Navier-Stokes strong form we need to provide the boundary conditions for the velocity field and the turbulent variables. We impose

\[
\mathbf{u} = 0 \text{ on } \partial \Omega, \quad k = 0 \text{ on } \partial \Omega, \quad \nabla \omega \cdot \hat{n} = 0 \text{ on } \partial \Omega,
\]

where \( \partial \Omega = \Gamma_C \cup \Gamma_B \cup \Gamma_R \cup \Gamma_T \) is the boundary of the domain \( \Omega \). We denote with \( \Gamma_C \) the controlled boundary corresponding to the hot wall, with \( \Gamma_T \) and \( \Gamma_B \) the top and bottom insulated walls and with \( \Gamma_R \) the cold wall. For the temperature field we set the following boundary conditions

\[
T = T_c \text{ on } \Gamma_R, \quad \nabla T \cdot \hat{n} = 0 \text{ on } \Gamma_B \cup \Gamma_T, \quad T = h \text{ on } \Gamma_C,
\]

where \( T_c \) is given and \( h \) is the optimal boundary temperature.

### 2.2. Boundary control and optimality system

In order to obtain the optimality system an objective functional has to be chosen. We study a boundary control problem with the aim of obtaining desired velocity profiles and of enhancing/reducing the turbulent energy \( k \). It is possible to express the problem in a mathematical form by the minimization of an objective or cost functional defined as

\[
\mathcal{J}(\mathbf{u}, k, h) = \frac{\alpha_u}{2} \int_{\Omega} ||\mathbf{u} - \mathbf{u}_d||^2 d\Omega + \frac{\alpha_k}{2} \int_{\Omega} |k - k_d|^2 d\Omega + \lambda \int_{\Gamma_C} |h|^2 d\Gamma + \gamma \int_{\Gamma_C} ||\nabla_s h||^2 d\Gamma, \quad (7)
\]

where \( \nabla_s \) denotes the surface gradient operator, defined as \( \nabla_s h = \nabla h - \hat{n} \mathbf{u} \cdot \nabla h \). The positive parameters \( \alpha_u, \alpha_k, \lambda \) and \( \gamma \) can be used to change the relative importance between objective and cost contributions, as well as to act as penalty parameters. The two first terms take into account the difference expressed in \( L^2(\Omega) \) norm between the fluid velocity field \( \mathbf{u} \) and its target profile \( \mathbf{u}_d \), as well as for the turbulent kinetic energy and its desired value \( k_d \). If \( \alpha_u = 0 \) a turbulent kinetic energy matching problem is considered; if \( \alpha_k = 0 \) a velocity matching case is studied. Terms containing \( \lambda \) and \( \gamma \) are penalization contributions introduced to limit the norm of the boundary control function \( h \) and its gradient. In this way, boundary control parameter is limited to Sobolev space \( H^1(\Gamma_C) \). The choice of the values of \( \lambda \) and \( \gamma \) is important for the solution of the optimal control problem since high values of penalization parameters \( \lambda, \gamma \rightarrow 0 \) can result in too smooth control and poor optimization while low values \( \lambda, \gamma \rightarrow 0 \) may lead to convergence issues in the numerical solution of the problem.

Since we are dealing with a constrained optimization, we can reformulate the minimization problem (7) with constraints (1)-(6) by employing the Lagrangian multipliers method [2]. The
The total Lagrangian can be written as
\[
L(u, p, k, \omega, \nu_t, T, h, u_a, p_a, k_a, \omega_a, \nu_a, T_a) = \mathcal{J}(u, k, h) + \int_\Omega p_a \nabla \cdot u \, d\Omega + 
\]
\[
+ \int_\Omega u_a \cdot [(u \cdot \nabla)u + \nabla p - \nabla \cdot [(\nu + \nu_t)S(u)] - \beta(T - T_{\text{ref}})g] \, d\Omega + 
\]
\[
+ \int_\Omega k_a \left\{ (u \cdot \nabla)k - \nabla \cdot [(\nu + \sigma_k \nu_t)\nabla k] - \frac{\nu_t}{2} ||S(u)||^2 + \beta_k \nu k - \frac{\nu_t}{Pr_t} g \cdot \nabla T \right\} \, d\Omega + 
\]
\[
+ \int_\Omega \omega_a \left\{ (u \cdot \nabla)\omega - \nabla \cdot [(\nu + \sigma_\omega \nu_t)\nabla \omega] - \frac{\omega}{2} ||S(u)||^2 + \beta_\omega \omega^2 - \frac{\beta \omega}{Pr_t} g \cdot \nabla T \right\} \, d\Omega + 
\]
\[
+ \int_\Omega \nu_a \left\{ (\nu_t - \frac{k}{\omega}) (\nu_t - \nu_{\text{max}}) \right\} \, d\Omega + \int_\Omega T_a \left\{ (u \cdot \nabla)T - \nabla \cdot \left[ (\alpha + \frac{\nu_t}{Pr_t}) \nabla T \right] \right\} \, d\Omega. 
\]

The total Lagrangian (8) includes the objective functional (7), the Reynolds Averaged energy and Navier-Stokes equations closed with the k-\omega turbulence model. We substitute \( \alpha_t \) with the expression (6) in order reduce the number of unknowns. By taking the Fréchet derivatives [14] of the Lagrangian with respect to every adjoint variable, the weak form of the state system is obtained. By setting the first variation of the Lagrangian functional with respect to the state variables equal to zero, the adjoint system in weak form can be written. Considering the variations with respect to pressure and velocity fields we obtain the adjoint continuity and adjoint Navier-Stokes equations
\[
\int_\Omega \nabla \cdot u_a \delta p \, d\Omega = 0, \quad \forall \delta p \in L^2(\Omega) 
\]
\[
\int_\Omega \left\{ [(u \cdot \nabla)u - u \cdot \nabla u_a - \nabla p_a] \cdot \delta u + (\nu + \nu_t) \nabla \delta u : \nabla u_a \right\} \, d\Omega = \int_\Omega \delta u \cdot [-k_a \nabla k + 
\]
\[- \omega_a \nabla \omega - T_a \nabla T + S(u)(k_a \nu_t + c_\omega \omega_a) - \alpha_a (u - u_d)] \, d\Omega \quad \forall \delta u \in H^1(\Omega). 
\]

Adjoint k-\omega equations are as follows
\[
\int_\Omega \left\{ -u \cdot \nabla k_a - \nabla \cdot [(\nu + \sigma_k \nu_t) \nabla k_a] \right\} \delta k \, d\Omega = \int_\Omega \frac{\nu_a}{\omega} (\nu_t - \nu_{\text{max}}) - \beta k \omega + 
\]
\[- \alpha_k (k - k_d) \right\} \delta k \, d\Omega, \quad \forall \delta k \in H^1(\Omega) 
\]
\[
\int_\Omega \left\{ -u \cdot \nabla \omega_a - \nabla \cdot [(\nu + \sigma_\omega \nu_t) \nabla \omega_a] \right\} \delta \omega \, d\Omega = \int_\Omega \left[ -\frac{\nu_a k}{\omega^2} (\nu_t - \nu_{\text{max}}) - \beta \omega k + 
\]
\[- 2 \beta_\omega \omega \right\} \delta \omega \, d\Omega, \quad \forall \delta \omega \in H^1(\Omega). 
\]

By imposing the Lagrangian variation with respect to the eddy viscosity to vanish, the algebraic adjoint eddy viscosity equation can be written as
\[
\nu_a (\nu_t - \nu_{\text{max}}) = \frac{k_a}{2} S(u) : S(u) - S(u) : S(u_a) - \sigma_k \nabla k \cdot \nabla k_a - \sigma_\omega \nabla \omega \cdot \nabla \omega_a + 
\]
\[- \frac{1}{Pr_t} \nabla T \cdot \nabla T_a + \frac{\beta}{Pr_t} k_a g \cdot \nabla T. 
\]

By considering the variations with respect to the temperature field, the adjoint temperature equation is obtained
\[
\int_\Omega \left\{ -u \cdot \nabla T_a \delta T + \left( \alpha + \frac{\nu_t}{Pr_t} \right) \nabla T_a \cdot \nabla \delta T \right\} \, d\Omega = \int_\Omega \beta g \cdot \left[ u_a \delta T + \frac{1}{Pr_t} \nabla \delta T (k_a \nu_t + \omega_a) \right] \, d\Omega + 
\]
\[
+ \int_{T_c} \left( \alpha + \frac{\nu_t}{Pr_t} \right) \nabla T_a \cdot \hat{n} \delta T \, d\Gamma, \quad \forall \delta T \in H^1(\Omega). 
\]
Finally, considering the variations $\delta h$ on the controls $h$ we have

$$
\int_{\Gamma_c} (\lambda h \delta h + \gamma \nabla h \cdot \nabla \delta h) \, d\Gamma = \int_{\Gamma_c} \left( \alpha + \frac{\nu h}{\mu T} \right) \nabla T_a \cdot \hat{n} \delta h \, d\Gamma \quad \forall \delta h \in H^1(\Gamma_c). \tag{15}
$$

In the case one might be interested in a finite volume discretization, it is necessary to recover the strong form of the adjoint system. Integrating by parts (9-12), (14) and (15) and imposing the surface contributions to vanish, it is possible to gain the strong form of the adjoint system completed by its boundary conditions reported in Table 1.

### 3. Numerical results

![Temperature and velocity fields](image)

**Figure 1.** Velocity matching case: temperature (a) and velocity (b) fields in an uncontrolled case. Temperature (c) and velocity (d) in the velocity matching case with $\lambda = 0.001$.  

To perform the numerical simulations, we use a finite element discretization of the optimality system written in weak form (9)-(15). We replace the infinite dimensional functional spaces by finite dimensional ones and proper basis for these spaces are chosen [12]. We use finite quadratic elements for all variables except the pressure which is assumed linear to satisfy the BBL $\inf$-$\sup$ stability condition. By doing that we obtain $u_h, u_{ah} \in X_h^2(\Omega) \subset H^1(\Omega), \ p_h, p_{ah} \in S_h(\Omega) \subset L^2(\Omega), \ k_h, k_{ah}, \omega_h, \omega_{ah}, T_h, T_{ah} \in X_h^2(\Omega) \subset H^1(\Omega)$ and $h \in X_h^2(\Gamma) \subset H^1(\Gamma)$.  

The optimality system cannot be solved with a one-shot method due to its strong non-linearity. Therefore we use a segregate approach and we apply the steepest descent method, a first order iterative algorithm for finding the minimum of a functional. The algorithm that we have implemented in the finite element in-house code FEMuS [15] is reported in Algorithm 1.
Figure 2. Turbulence enhancement case: temperature (a), turbulent energy (b) and velocity (c) fields in an uncontrolled case. Temperature (d), turbulent energy (e) and velocity (f) in the turbulence enhancement case with $\lambda = 0.0001$.

Figure 3. Velocity matching case: velocity $u_x$ in a line at $y = 0.008m$ with $\lambda$ varying and $\gamma = 0$ (a), with $\gamma$ varying and $\lambda = 10^{-5}$ (c); boundary temperature on $\Gamma_c$ for tests with $\lambda$ varying and $\gamma = 0$ (b), with $\gamma$ varying and $\lambda = 10^{-5}$ (d). The solid line represents uncontrolled solutions ($\lambda \rightarrow \infty$) in (a) and (b), $L^2(\Gamma)$ solution in (c) and (d).

The geometry we have considered is a square cavity with $L = 0.01m$. We set on $\Gamma_C$ a
temperature $h^0 = 283K$ while $T = 273K$ on $\Gamma_R$, as shown in Figure 1(a). Air flows in the cavity due to buoyancy forces caused by the heated cavity walls and the velocity field is reported in Figure 1(b).

First a velocity matching case is considered. Let be $\Omega_d = [0.0030; 0.0070] \times [0.0070; 0.0090]$ the region where we aim to minimize the objective functional with $\alpha_u = \chi_{\Omega_d}$ and $\alpha_k = 0$. The uncontrolled average $u_x$ results 0.0074m/s in $\Omega_d$ and we choose a uniform velocity profile as desired velocity, i.e. $u_d = (0.01, 0)m/s$. We now perform many tests changing the regularization parameters $\lambda = 10^{-1}, 10^{-2}, 10^{-3}$ and $\gamma = 10^{-8}, 10^{-9}, 10^{-10}$.

In order to analyze the influence of the $L^2(\Gamma)$ regularization parameter $\lambda$, we show results with $\gamma = 0$ and different $\lambda$ values in Figures 3(a) and 3(b). When $\lambda$ is small the control can act strongly and the boundary temperature profile is more irregular and harder to be reproduced from the numerical point of view, as one can see in Figure 3 (b) and 1(c). Meanwhile, Figure 1(d) and 3 (a) shows how a smaller value of $\lambda$ provides a better matching with the objective. When $\lambda = 0.1$ the control is very weak and the optimal solution is close to the reference state corresponding to $\lambda \to \infty$. In the central region, as $\lambda$ decreases, the velocity approaches the desired value and the matching is better achieved. Due to the vanishing boundary conditions set on the walls, the control cannot act efficiently in the near wall region, where the velocity is farther from the desired mean value.
In Figure 3 (c) and (d) the optimal solution dependence on the control parameter $\gamma$ is shown. We set $\lambda = 10^{-3}$ and we study $\gamma$ influence on the control parameter. Figure 3 (c) evidences that the highest value of $\gamma$ among the considered ones leads to a very poor control and an optimal solution very close to the uncontrolled state. Limiting the control parameter $H^1(\Gamma)$ norm implies severe limits on the size of the function and its gradient. Therefore only smooth and regular solutions can be accepted. When low values of $\gamma$ are considered, the boundary control parameter is closer to the solution obtained with $\gamma = 0$.

We also show the results of a turbulence enhancement case with different $\lambda$ values. Let be $\Omega_d = [0.0020; 0.0040] \times [0.0020; 0.0050]$ the region where the objective is considered. As one can note in Figure 2 (e) the variable $k$ assumes values below $2.7 \cdot 10^{-7} m^2/s^2$ in the region $\Omega_d$, therefore we set $10^{-5} m^2/s^2$ as desired value. Now we study the dependence of the solution on the regularization parameter $\lambda$, as shown in Figure 4, testing the values $\lambda = 10^{-3}, 5 \cdot 10^{-4}$ and $10^{-4}$. As in the previous tests, for low values of $\lambda$ the control is more efficient and effective. Turbulent kinetic energy and velocity fields are shown in Figures 2 (e) and (f) for the lowest $\lambda$ case. Nevertheless, the boundary control parameter achieved is not smooth, as reported in Figure 2 (d). In these tests we consider $\lambda$ values lower than those considered for the velocity matching case, because the adjoint temperature dependence on the adjoint turbulent kinetic energy is not as strong as evaluated in (14).

4. Conclusions
An adjoint-based boundary optimal control method for the Reynolds Averaged energy and Navier-Stokes equations coupled with a two-equations turbulence model has been presented. Considered problems class is characterized by a strong coupling between velocity and temperature fields due to buoyancy forces and advection, therefore it is possible to control the flow by acting on the temperature field and vice versa. Adjoint system has been obtained through a Lagrangian functional minimization. Proper boundary conditions have been set on the adjoint variables and a steepest descent algorithm has been implemented for the segregate solution of the optimality system. Simple test cases have been reported to show the robustness of the mathematical approach presented for different objectives and different regularizations.

References
[1] ANSYS 2012 ANSYS FLUENT 14.5 - Theory Guide, Optimization feature, Morpher-Optimization feature (ANSYS, Inc., Canonsburg, PA, USA)
[2] Gunzburger M D 2003 Perspectives in flow control and optimization vol 5 (Siam)
[3] Lee H C and Kim S 2004 J. Korean Math. Soc 41 681–715
[4] Lee H C and Imanuvilov O Y 2000 Journal of mathematical analysis and applications 242 191–211
[5] Aulisa E, Bornia G and Manservisi S 2015 Commun. Comput. Phys. 189(3) 621–649
[6] Lee H C and Shin B C 2000 Mathematical methods in the applied sciences 23 227–254
[7] Lee H C and Choi Y 2006 Computers & Mathematics with Applications 51 829–848
[8] Gunzburger M and Manservisi S 2000 Comput Methods Appl Mech Eng 189(3) 803–823
[9] Chirico L, Chierici A, Da Vià R, Giovacchini V and Manservisi S 2019 Journal of Physics: Conference Series vol 1224 (IOP Publishing) p 012006
[10] Manservisi S and Menghini F 2016 Computers & Fluids 125 130–143
[11] Manservisi S and Menghini F 2016 Computers & Mathematics with Applications 71 2389–2406
[12] Brenner S and Scott R 2007 The mathematical theory of finite element methods vol 15 (Springer Science)
[13] Da Vià R 2019 Development of a computational platform for the simulation of low Prandtl number turbulent flows Ph.D. thesis University of Bologna
[14] Tröltzsch F 2010 Optimal control of partial differential equations: theory, methods, and applications vol 112 (American Mathematical Soc.)
[15] Code FEMuS URL https://github.com/FemusPlatform/femus