

Towards the LES Simulation of IC Engines with Parallel Topologically Changing Meshes

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ABSTRACT

The implementation and the combination of advanced boundary conditions and subgrid scale models for Large Eddy Simulation (LES) in the multi-dimensional open-source CFD code OpenFOAM® are presented. The goal is to perform reliable cold flow LES simulations in complex geometries, such as in the cylinders of internal combustion engines. The implementation of a boundary condition for synthetic turbulence generation upstream of the valve port and of the compressible formulation of the Wall-Adapting Local Eddy-viscosity sgs model (WALE) is described. The WALE model is based on the square of the velocity gradient tensor and it accounts for the effects of both the strain and the rotation rate of the smallest resolved turbulent fluctuations and it recovers the proper y^3 near-wall scaling for the eddy viscosity without requiring dynamic procedure; hence, it is supposed to be a very reliable model for ICE simulation. Validation of the implemented models has been performed separately on two steady state flow benches, where experimental data were available: a backward facing step geometry and a simple IC engine geometry with one axed central valve. A method to evaluate the turbulence resolution of LES simulation based on a Length Scale Resolution (LSR) parameter has been proposed and a discussion about the completeness of the LES simulation (i.e. LES simulation quality) is presented. Finally, the implementation of a fully parallel algorithm for the management of topologically changing meshes in the OpenFOAM®-2.1.x technology is described. The aim is to implement a reliable framework to perform LES simulation of internal combustion engines by the OpenFOAM® technology.

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INTRODUCTION

Numerical simulation represents nowadays a very common approach to improve the understanding of the complex physical phenomena occurring in Internal Combustion (IC) Engines. A correct modeling of the turbulent motion is very important to achieve reliable predictions of the gas exchange phase (swirl, tumble), of fuel mixing and combustion, of the cyclic combustion variability. In CFD engine simulation, the most widely used approach is the Reynolds Averaged Navier-Stokes (RANS) method. In RANS, the turbulence effects are taken into account without the direct solution of the turbulent structure but only by adopting specific turbulence models acting on the flow viscosity [1, 2]. If the turbulent flow is modeled without directly solving the turbulence structures, the computational cost results to be drastically reduced and, at the same time, an acceptable accuracy to reproduce the mean engine flow characteristics may be achieved. The main drawback of the RANS approach lies in the impossibility to correctly predict

the unsteady behavior of the turbulent flow into the engine. In this context, the numerical representation of the turbulence is a fundamental aspect for the overall quality of an IC-Engine CFD simulation. From this point of view, Large Eddy Simulation (LES) applied to ICE is potentially a reliable tool to simulate turbulent motion in the engine cycle. In LES, the Navier-Stokes equations are filtered in space, allowing a separation of the turbulent scales between Grid-Scales (GS) and Sub-Grid Scales (SGS). The GS part corresponds to the resolved large-scales of motion responsible for the momentum, heat, and mass transfer in separated or free shear flow regions. The SGS part corresponds to the more statistically isotropic and universal small not resolved residual motions. Despite the application of LES to IC-Engine simulation looks promising, there are some known issues that cannot be neglected. First, boundary conditions in LES must be able to properly handle both acoustic waves and turbulence properties. Then, the discrete solution of the Navier Stokes equations on unstructured meshes, typically used for real-world IC-engine applications, may lead to a

numerical dissipation that is comparable to the eddy viscosity ν_{sgs} . Moreover, when simulations of complex geometries such as in IC engines are performed, also the near-wall behavior of the eddy-viscosity represents a further difficulty [3].

This paper is divided in two main parts. In the first part, a boundary condition for synthetic turbulence generation at inlet boundary is presented together with the implementation of the WALE SGS model [4] in its compressible formulation. In the second part, the implemented LES models have been used to predict the flow conditions over two test cases: a backward facing step geometry [5] and a like IC-Engine configuration [6]. For both cases, results from compressible LES simulation have been compared to experimental LDA measurements. The quality of the performed LES simulations are evaluated by the Length Scale Resolution (LSR) parameter defined by the authors [7, 8]. All the models described have been implemented in Lib-ICER[®], a C++ library based on the OpenFOAM[®] technology [9, 10, 11, 12]. Finally, a fully parallel algorithm for topologically changing meshes has been developed in the OpenFOAM[®]-2.1.x technology and it is presented. The aim is to build up a framework in the OpenFOAM[®]-2.1.x technology for complete LES simulation of IC engines.

As it will be shown further, compressible models were validated on cases where the flow could be considered as incompressible. While this choice is clearly not computationally efficient, it was driven by the need to validate the implementation of the compressible models (needed in the simulation of IC engines) by reliable experimental results available from the literature. The validation of the models developed for the incompressible case has been validated by the authors in [8].

SYNTHETIC TURBULENCE INLET B.C.

In a Large Eddy Simulation, the velocity field at the inflow must be as close as possible to a “real” turbulent flow. In particular, it must reflect the salient characteristics of turbulence (like randomness, time- and space-correlation, and solenoidality), and it must correspond to the real flow with respect to some statistics (mean velocity, energy spectrum, lengthscales, etc.) [3, 13]. One way to obtain “turbulent-like” velocity at the inlet is to artificially generate synthetic fluctuations with the desired characteristics, and superpose them onto a mean velocity profile [14]. As first step, the fluctuating component of the velocity is generated as a sum of Fourier modes:

$$u_i''(x_j) = 2 \sum_{n=1}^N \hat{u}^n \cos(\kappa_j^n x_j + \psi^n) \sigma_i^n \quad (1)$$

where $\hat{u}^n$, ψ^n are the amplitude and phase of Fourier mode n ; κ_j^n is the corresponding wavenumber vector, that is oriented

in space according to angles θ^n and φ^n , and it ranges from k_1 to k_N . Finally, σ_j^n is the unit velocity vector of κ_j^n (see Fig. 1).

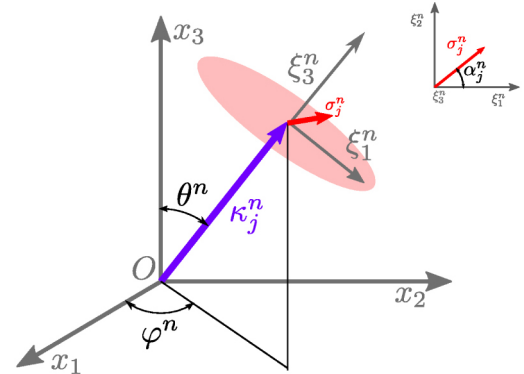


Figure 1. Illustration of the symbols used in Eq. (1). The wavenumber velocity σ_j^n must lie in a plane orthogonal to the wavenumber vector κ_j^n to ensure solenoidality of the velocity field [14].

In order to avoid that the generated fluctuations are destroyed by the Navier-Stokes solver, solenoidality of the velocity field must be enforced; this can be achieved by ensuring that the velocity vector σ_j^n lies in a plane orthogonal to κ_j^n [14]. The angle α^n is the orientation of σ_j^n on the (ξ_1, ξ_2) plane, as shown in Fig. 1. Geometric angles ϕ_n , α_n and θ_n and phase angle ψ_n are random variables; they are generated for each mode n according to a given statistical distribution (see Tab. 1). Spectral mode amplitude $\hat{u}^n$ is calculated according to a prescribed spectrum shape $E(\kappa)$: $\hat{u}^n = \sqrt{E(\kappa)}$. In this work, a modified version of the Von Kármán energy spectrum has been used:

$$E(\kappa) = A \frac{u_{rms}^2}{\kappa_e} \frac{(\kappa/\kappa_e)^4}{[1 + (\kappa/\kappa_e)^2]^{17/6}} \exp[-2(\kappa/\kappa_e)^2]$$

where:

- $\kappa_e = 2\pi/\eta$ corresponds to Kolmogorov lengthscale $\eta = \nu^{3/4} \varepsilon^{-1/4}$
- $A = 1.456$ is a model's constant
- $\kappa_e = 9\pi/55 A/\mathcal{L}$ is a function of the integral length-scale ($\mathcal{L}$).

Table 1. Statistical distribution of angles φ^n , ψ^n , θ^n and α^n .

$\mathcal{P}(\varphi^n) = 1/(2\pi)$	$0 \leq \varphi^n \leq 2\pi$
$\mathcal{P}(\psi^n) = 1/(2\pi)$	$0 \leq \psi^n \leq 2\pi$
$\mathcal{P}(\theta^n) = 1/\sin(\theta)$	$0 \leq \theta^n \leq \pi$
$\mathcal{P}(\alpha^n) = 1/(2\pi)$	$0 \leq \alpha^n \leq 2\pi$

The highest wave number of the artificial spectrum is taken as the spatial filter cutoff frequency, that is a function of the filter width: $k_{max} = 2\pi/(\Delta\mathcal{L})$. Conversely, the smallest

wave number is defined from $k_1 = k_e/p$, where k_e corresponds to the energy-carrying eddies lengthscale. Factor p should be larger than one to make the largest scales larger than those corresponding to k_e . In the present work $p = 2$ [14]. The wavenumber space, $k_{max} - k_1$ is divided into N modes (typically 150-600), equally spaced, of size Δk . If turbulence has to be generated for channel flow case, k_η can be calculated as $k_\eta = 2\pi/(Re_y^{-3/4})$.

A fluctuating velocity field is then generated for each time step as described above. Fields generated at different timesteps are however independent of each other, and their time correlation is thus zero: this is unphysical. To enforce correlation in time, the new fluctuating velocity field, u'_i is weighted with the previous one on the basis of an asymmetric time filter [15].

$$(u')^m = a(u')^{m-1} + b(u'')^m \quad (3)$$

where ($\mathcal{T}$ is the integral timescale):

$$a = \exp(-\Delta t/\mathcal{T}), \quad b = \sqrt{1-a^2}$$

In the simulations, the mean inlet profiles are either set from experiments or, for example, from the law of the wall. The synthetic fluctuations created yield isotropic turbulence in the inlet plane: u_{rms} , v_{rms} and w_{rms} are constant in time, though they vary with the distance from solid walls. The algorithm for synthetic turbulence generation is applied at each temporal integration step, leading to a small increase of the total simulation time.

The WALE SGS Stress Tensor Model

In this work, the WALE (Wall-Adapting Local Eddy-viscosity) model [4] has been implemented in its compressible formulation. The model is based on the eddy-viscosity assumption:

$$\tau_{ij}^{SGS} = \mu_t \left(2\tilde{S}_{ij} - \frac{2}{3}\tilde{S}_{mm}\delta_{ij} \right) - \frac{2}{3}\tilde{\rho}k^{SGS}\delta_{ij} \quad (4)$$

where τ_{ij} is the subgrid scale viscous stress tensor and $\tilde{S}_{ij}$ is the Favre-filtered strain rate tensor

$$\tilde{S}_{ij} = \frac{1}{2} \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) \quad (5)$$

The overbar denotes space filtered quantities (implicitly performed by the computational grid), while the tilde denotes the Favre-filtered quantities. For most of the eddy-viscosity models, the eddy-viscosity can be written in the general formulation:

$$\mu_{sgs} = C_m^2 \bar{\rho} \Delta^2 \tilde{OP}(\mathbf{x}, t) \quad (6)$$

where C_m is the constant of the model, Δ is the subgrid characteristic length scale and $\tilde{OP}$ is an operator of space and time, homogeneous to a frequency, defined from the resolved fields. If compared to the dynamic formulation of the Smagorinsky model [16], the WALE model includes in the incompressible formulation of the operator $\tilde{OP}$ the traceless symmetric part of the square of the gradient velocity tensor $\tilde{g}_{ij} = \frac{\partial u_i}{\partial x_j}$:

$$\begin{aligned} s_{ij}^d &= \frac{1}{2} (\tilde{g}_{ij}^2 + \tilde{g}_{ji}^2) - \frac{1}{3} \delta_{ij} \tilde{g}_{kk}^2 \\ &= \tilde{S}_{ik} \tilde{S}_{kj} + \tilde{\Omega}_{ik} \tilde{\Omega}_{kj} - \frac{1}{3} \delta_{ij} [\tilde{S}_{mn} \tilde{S}_{mn} - \tilde{\Omega}_{mn} \tilde{\Omega}_{mn}] \end{aligned} \quad (7)$$

where $\tilde{g}_{ij}^2 = \tilde{g}_{ik} \cdot \tilde{g}_{kj}$ and δ_{ij} is the Kronecker symbol, Ω is the anti-symmetric part of $\tilde{g}$ (or, the vorticity tensor):

$$\tilde{\Omega}_{ij} = \frac{1}{2} \left(\frac{\partial \tilde{u}_i}{\partial x_j} - \frac{\partial \tilde{u}_j}{\partial x_i} \right) \quad (8)$$

By construction, the trace of s^d is zero and its second invariant remains finite and proportional to $s_{ij}^d s_{ij}^d$, so that for the incompressible case:

$$s_{ij}^d s_{ij}^d = \frac{1}{6} (S^2 S^2 + \Omega^2 \Omega^2) + \frac{2}{3} S^2 \Omega^2 + 2IV_{S\Omega} \quad (9)$$

where

$$S^2 = \tilde{S}_{ij} \tilde{S}_{ij} \quad \Omega^2 = \tilde{\Omega}_{ij} \tilde{\Omega}_{ij} \quad IV_{S\Omega} = \tilde{S}_{ik} \tilde{S}_{kj} \tilde{\Omega}_{jl} \tilde{\Omega}_{li}$$

Since with the WALE model the invariant $\tilde{S}_{ij} \tilde{S}_{ij}$ is zero in the case of pure shear, the model is able to reproduce the laminar to turbulent transition. The formulation of the WALE model is based on the operator $s_{ij}^d s_{ij}^d$ and this represents its main advantage with respect to the dynamic Smagorinsky model, since it is sensitive to both the strain and the rotation rate of the small turbulent structures. Because of this, it is well suited for LES in complex geometries with structured or unstructured methods because no explicit filtering is needed and only local information is required to build the eddy-viscosity. This is achieved by the definition of an operator $\tilde{OP}$ with the following properties:

- invariant to any coordinate translation or rotation
- easily assessed on any kind of computational grid
- function of both the strain and the rotation rates

• it goes naturally to zero at the wall so that neither damping function nor dynamic procedure are needed to reproduce the effect of the no-slip condition

For the compressible case, the resulting formulation for the eddy viscosity then is:

$$\mu_t = \bar{\rho} (C_w \Delta)^2 \frac{\tilde{O}P_1}{\tilde{O}P_2} = \bar{\rho} (C_w \Delta)^2 \frac{(s_{ij}^d s_{ij}^d)^{\frac{3}{2}}}{(\tilde{S}_{ij} \tilde{S}_{ij})^{5/2} + (s_{ij}^d s_{ij}^d)^{5/4}} \quad (10)$$

In Eq. (10), the ratio $\tilde{O}P_1/(\tilde{S}_{ij} \tilde{S}_{ij})^{5/2}$ ensures to keep the y^3 behavior of the whole operator near the wall and to have a formulation of operator consistent with Eq. (6). At the same time, $\tilde{O}P_1/(\tilde{S}_{ij} \tilde{S}_{ij})^{5/2}$ is not well conditioned numerically since the denominator can locally tend to zero while $\tilde{O}P_1$ remains finite. The way used in [4] to avoid this situation is to scale $\tilde{O}P_1$ by $(\tilde{S}_{ij} \tilde{S}_{ij})^{5/2} + (s_{ij}^d s_{ij}^d)^{5/4}$; the second term in the denominator is negligible near the wall but it avoids numerical instabilities because $\tilde{O}P_2$ does not go to zero for pure shear or irrotational strain. Although the dynamic procedure could also be applied to the WALE model, in this work C_w has been considered as a true constant, assessed from the case of isotropic homogeneous turbulence [4].

In order to write the subgrid-scale viscous stress tensor, the relation between the turbulent viscosity ν_t (see Eq. 6) and the turbulent subgrid scale kinetic energy k^{sgs} must be considered:

$$k^{sgs} = C_2 \Delta^2 \tilde{S}_{mn} \tilde{S}_{mn} = C_2 \Delta^2 \left(\frac{\mu_t}{\bar{\rho} C_m^2 \Delta^2} \right)^2 = C_w' \left(\frac{\mu_t}{\bar{\rho} \Delta} \right)^2 \quad (11)$$

By the combination of Eq. (11) and Eq. (4) it follows:

$$\tau_{ij}^{SGS} = 2\mu_t \left(\tilde{S}_{ij} - \frac{1}{3} \tilde{S}_{mm} \delta_{ij} \right) - \frac{2}{3} \frac{C_w'}{\bar{\rho}} \left(\frac{\mu_t}{\Delta} \right)^2 \delta_{ij} \quad (12)$$

As suggested in [17], C_w' has been set to 45.8. To make the stress realizable, its diagonal entries were forced to be nonpositive.

ANALYSIS AND DISCUSSION OF THE RESULTS

A validation study for the implementation of the proposed models and of the simulation methodology has been applied on the backward-facing step (BFS) test-case [5], for which an extensive set of experimental measurements was available. Moreover, it has features that make it a good validation test case for engines, since it includes phenomena that are similar to the ones occurring during the intake stroke of the engine, when air flows to the combustion chamber through the valve

ports. Finally, to explore the suitability of the proposed approach for reciprocating internal combustion engines, a simplified IC geometry with one axis-centered valve [6] has been simulated.

The main goal of a LES simulation is to directly solve all the non-isotropic turbulent scales over the inertial sub-range. Therefore, the quality of a LES simulation can be directly referred to the evaluation of the flow turbulent energy budget directly solved during the simulation itself. To measure the LES simulation resolution, Pope [18] proposed to adopt the so called M parameter defined as:

$$M = \frac{k_{sgs}(\mathbf{x}; t)}{k_{sgs}(\mathbf{x}; t) + K(\mathbf{x}; t)} \quad (13)$$

where $K(\mathbf{x}; t)$ is the kinetic energy of the resolved (grid) motion and $k_{sgs}(\mathbf{x}; t)$ is the kinetic energy of the unresolved (subgrid) scales. M is always bounded between 0.0 and 1.0 (0.0=DNS simulation; 1.0=RANS simulation). In principle, the M parameter is a very useful tool to evaluate the energy resolution level but the link between M value and the local filter size (i.e. to the local cell characteristic dimension) is not apparent.

An alternative method to evaluate the turbulence resolution for a LES simulation is to use the *Length Scale Resolution* (LSR) parameter defined by authors as:

$$LSR = \frac{\Delta}{\ell_{di}} \quad (14)$$

where Δ is the local filter size and ℓ_{di} is the lower limit of the inertial sub-range:

$$\ell_{di} = 60\eta \quad (15)$$

where η is the Kolmogorov scale [18]. The LSR parameter is proportional to the deviation between the actual resolved energy level and the corresponding lower limit of the inertial sub-range. Where the LSR value is equal to 1 all the turbulent scales up to the viscosity range are resolved. By the LSR definition, the evaluation of the actual resolved energy level is directly linked to the local filter size. It helps to clearly match the adopted mesh size to the local energy resolution all over the computational domain. In [7, 19, 8], authors found that a LSR value of 3-5 is the upper limit to guarantee a reasonable LES resolution at an affordable computational cost. As it was found in [8] and as it will be shown further in this work, the LSR parameter provides reliable information about the completeness of the LES simulation, provided that the meshes are generated with the same strategy (in terms of cell distribution and shape).

Backward Facing Step Geometry

The single-side expansion of Fig. 2-a was considered in this study. The results obtained by LES for mean velocity

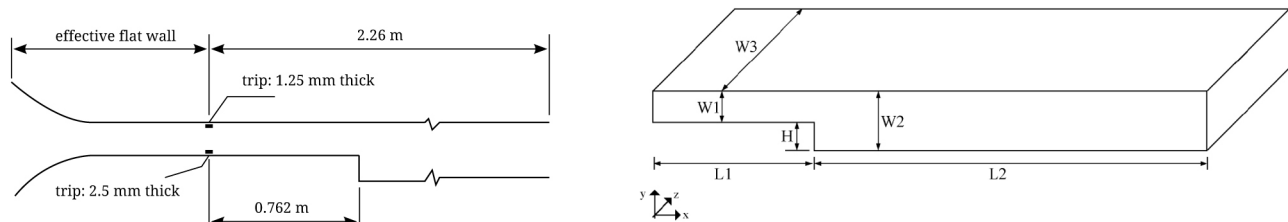


Figure 2. a) Experimental setup of the backward facing step geometry by Eaton et al. [5]. b) Schematic of the backward facing step geometry simulated [5]; $L_1 = 0.4953$ m; $L_2 = 1.55$ m; $W_1 = 0.0762$ m; $W_2 = 0.127$ m; $W_3 = 0.015$ m, $H = 0.0508$ m.

profiles and for velocity fluctuations have been quantitatively compared to the experimental measurements by hot-wire anemometry performed by Eaton et al. [5] in terms of both mean and RMS velocities. In the experiments, the turbulent boundary layer was generated in the inlet channel of the backward facing step by positioning two trips, that were placed at the same distance from the step: the first one was located on the bottom wall and the second one on the top wall.

Trips heights were 2.5 mm and 1.25 mm respectively; the boundary layer thickness on the walls was therefore different. The inlet stream, at $Re = 40000$ (based on the bulk velocity U_0 at the inflow) was turbulent and fully developed at the step. In the simulations, only a small portion of the domain of the BFS was modeled, as shown in Fig. 2-b; the inlet channel length L_1 was chosen to have fully developed flow near the step, while the outlet channel length L_2 was chosen long enough to not have the numerical solution affected by the vicinity of the outlet boundary. Ambient pressure and temperature were used ($p = 101325$ Pa, $T = 298$ K); the working flow was air, with constant dynamic viscosity ($\mu = 1.9 \cdot 10^{-5}$ Pa s).

Table 2. Resolution of the meshes used for the simulations of the BFS geometry.

	Coarse	Fine
n. of cells	~ 1.2 M	~ 2.2 M
Δx_{max}^+	350	150
Δy_{max}^+	~ 1	0.1
Δz_{max}^+	60	60

Computational Procedure for BFS

In the present case a two-block orthogonal, fully-structured mesh system was used, with one block covering the upstream channel and the other one covering the downstream channel of the BFS. Simulations were carried out by an open-source CFD code [20], based on the finite volume approach. Second-order central differencing schemes in space for advection and diffusion were blended with linear-upwind schemes to stabilise solutions while maintaining second-order behavior [?]. The schemes applied result to be fully conservative and since the coefficients are always positive they are unconditionally bounded. Also, they satisfy the transportiveness requirement for large values of

local (cell) Peclet numbers. Unfortunately, no higher order schemes can be applied in the FV context when unstructured grids are used [?]. Time-marching was implicit, with the time derivative being discretised by a second-order backward approximation. The flux terms were advanced explicitly; the provisional velocity field was then corrected via the pressure gradient by a projection onto a divergence-free velocity field; pressure was computed as a solution to the pressure-Poisson problem. In order to improve the global convergence of the simulation, the operator splitting technique for pressure-velocity coupling was implemented as a *transient-SIMPLE* algorithm [2], where convergence of pressure-velocity solution is enforced by iterating the coupling procedure for each time step; the resulting fluid-dynamic CFL number, defined as $CFL = |u|\Delta t/\Delta x$, has been set to 5, with significant advantages in terms of required wall time. The code and the developed libraries were fully parallelised. The fluid-dynamic information recorded by a RANS simulation on a precursor domain has been used to reconstruct the turbulent fluctuations at the boundary inlet by the synthetic turbulence inlet b.c. described in Sec. ??.

A non-reflecting NSCBC-based boundary condition [9, 10] has been used at the outlet end. Walls were set as adiabatic. The subgrid stress tensor has been modeled by the compressible WALE model [4] and by the dynamic Smagorinsky model [16], already implemented by the authors [21]. The WALE model makes use of a constant C_w that is flow-dependent. In the simulations presented in this work, an average value of $C_w = 0.58$ has been taken from the literature, since it has been demonstrated that it is not significantly varying for very different types of flows [4]. Since both the dynamic Smagorinsky and the WALE model are self-adapting in the vicinity of solid walls, no wall functions were applied and flow equations were solved up to $y^+ \rightarrow 0$. The BFS domain was discretised by two different meshes, having 1.2 M (case “coarse”) and 2.2 M cells (case “fine”) respectively. This is in agreement with the studies of other authors [22].

Grids are the outcome of precursor testing. Local refinement was used near the walls to ensure the maximum value of y^+ within the limits reported in Tab. 2. In both cases, the width of the computational domain in the spanwise direction was set to $2H$ and cell-aspect ratio along the spanwise direction was maintained constant for the two cases.