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Predicting the total wall time of CFD simulations of single-compartment fires

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Abstract. The total wall time is often difficult to predict a priori in compartment fire simulations due to dynamic phenomena that can occur, e.g., flame extinction. The wall time is dependent on multiple physical factors in the simulation, along with simulation factors and the system used to compute the model. Specifically, the CFL number of a simulation is highly influential to the wall time, as this restricts the time step size. In this paper, the prediction of the total wall time for a single-compartment fire is investigated considering varying fire heat release rates and compartment ventilation factors. It is shown that an increasing heat release rate increases the total wall time due to higher velocities inside the compartment. Furthermore, when the compartment becomes under-ventilated, the wall time becomes more difficult to predict early on in the simulation, as steady state conditions are reached later, compared to well-ventilated cases. The time at which the wall time can be accurately predicted changed from a few physical seconds in the well-ventilated case, to up to 60 physical seconds for the under-ventilated case.

1. Introduction

One tool to investigate the fire safety in complex buildings is the use of Computational Fluid Dynamics (CFD), with the Fire Dynamics Simulator (FDS) [1] being a widely used CFD code. In general, it can take a significant amount of time to setup and compute complex cases with CFD, due to the complexity of creating, computing, and analysing a fire scenario and the CFD outputs.

The wall time of a simulation (i.e., the time it takes to complete computing the simulation) is often associated with the cost of the cloud services or High-Performance Computing (HPC) facilities, and its accurate prediction can, therefore, reduce the uncertainty associated with the costs of this service, or allow for better allocations of computational resources. As regards to fire simulations, the wall time of a simulation can depend on various factors, such as the total number of computational cells, the size of the time step, the heat release rate (HRR), combustion chemistry, etc. Furthermore, the wall time also depends on the specific individual computer and, in general, the computational resources used, which can have many parameters that influence the wall time, for instance processor speed and number of cores.

In previous studies, the prediction of the execution time has been investigated for various simple cases using historical data, where the cost execution time of a task is estimated using different machine learning or genetic algorithms [2-5]. For more complex scenarios, such as in CFD and HPC optimization, machine learning, combined with historical data to train the algorithms, has been used in a few applications [6-7]. As fire simulations are complex and involve multi-physical phenomena, the estimation of the total wall time of the simulations is difficult using these procedures, since large amounts of data must be generated to train algorithms. Another approach is to estimate the wall time during runtime. Predicting the wall time during runtime for a FDS simulation is shown in GitHub repository by Kris Overholt [8], but an analysis of this approach is not presented in the repository.

In CFD simulations, the wall time is typically dependent on the timestep which then depends on the individual simulation. A proposed constraint on the timestep is based on Courant-Friedrich-Lewy (CFL) number [9]:

$$CFL = \delta t \frac{||\boldsymbol{u}||}{\Delta} < 1 \quad (1)$$

where δt (s) is the time step size, $\boldsymbol{u}$ (m s^{-1}) is the velocity vector and Δ (m) is the cell width. The CFL number is advised to be between 0.8 to 1.0 in FDS simulations [9], meaning that a flow element is constrained – it cannot move more than the size of one control volume during a single time step. The velocity of this flow element can be calculated using different norms, with the default norm being the L_1-norm [9], see equation (2). This norm is the default, as it is the most restrictive, and, therefore, less prone to numerical instabilities, which would cause the results of the simulation to be unreliable.

$$\frac{||\boldsymbol{u}||}{\Delta} = \frac{|u|}{\delta x} + \frac{|v|}{\delta y} + \frac{|w|}{\delta z} + |\nabla \boldsymbol{u}| \quad (2)$$

where $|u|$ is the norm of velocity vector in the x-direction, $|v|$ is the norm of velocity vector in the y-direction, $|w|$ is the norm of velocity vector in the z-direction, and $|\nabla \boldsymbol{u}|$ is the divergence of the velocity vector. Since the size of the time step is governed by the CFL constraint and the velocity of the flow element, the size of the time step will vary throughout the simulation due to transient phenomena.

This paper investigates the possibility of predicting the wall time during runtime for well- and under-ventilated compartments, and whether an accurate prediction of the total wall time can be determined from the early stages of a simulation.

2. Methodology

The CFD code Fire Dynamics Simulator (FDS) version 6.8.0 is used, which is developed by the National Institute of Standards and Technology [1] and is continuously validated [12] for different fire scenarios. The CFD code uses the low Mach number assumption to solve the governing equations for fluid flow and energy transport. Turbulence is modelled using the Large Eddy Simulation (LES) approach, effectively resolving eddies which are larger than the chosen grid size, while the contribution from the smaller eddies is approximated with the use of a sub-grid scale model, in this case, the modified Deardorff model. Combustion is considered to be infinitely fast, based on a mixing-limited model [15], while turbulence-chemistry interactions are modelled with the Eddy Dissipation Concept (EDC). Radiation is modelled using the Finite Volume Method while the calculation of the absorption coefficients is based on a grey gas assumption. The study uses the default FDS models, along with their default model parameters.

The compartment experiments from Bouaza *et al.* [10], investigating the oscillatory burning regime in a cubic compartment (see Figure 1), are considered as a target test case of the simulations due to the compartment being well-defined and the availability of experimental results. A cubical computational domain, with a side length of 1.4 m, is used to model the scenarios in FDS. Cubic cells of 2 cm cell size in a single mesh have been used for all simulations similar to [11], with the mesh extended for 1 meter outside of the compartment at the opening.

The compartment walls are made of 20 cm thick cellular concrete with a density of $\rho = 450$ kg m^{-3}, a conductivity of $k = 0.11$ W m^{-1} K^{-1} and a specific heat capacity of $c_p = 1000$ J kg^{-1} K^{-1}. The fire source is a propane-fuelled square burner of 0.16 m side length, with a soot yield of 0.015, positioned in the centre of the compartment. The burner is flush to the floor with constant heat release rates of 100, 200, 300, 400 and 500 kW throughout the simulations. Each scenario is simulated for a total of 120 seconds, which is chosen to allow for all the simulations to reach steady-state conditions. A single ventilation opening of two different sizes (i.e., 0.8 m x 1.0 m and 0.2 m x 0.8 m) is considered to investigate how the wall time is influenced by going from well-ventilated to under-ventilated conditions inside the compartment. The classification of under-ventilated or well-ventilated compartments is based on Bouaza *et al.* [11] and is given by equation (3).

$$\dot{Q}_{in}^{max} = K\,A\,\sqrt{H} \tag{3}$$

where $\dot{Q}_{in}^{max}$ (kW) is the maximum fire heat release rate inside the compartment for ventilation-controlled conditions, K (kW m$^{-5/2}$) is a constant, A (m^2) is the opening area and H (m) is the opening height. The product $A\sqrt{H}$ (m$^{5/2}$) is known as the compartment ventilation factor and it is equal to 0.8 and 0.1 m$^{5/2}$ for the larger and smaller opening, respectively. In [11], the reported value for the constant K was between 850 to 1300. Assuming a constant value of 1300 kW m$^{-5/2}$, this yields 1040 kW and 133 kW for $\dot{Q}_{in}^{max}$, for the large and small opening, respectively. This means, that most cases with the small opening will be under-ventilated.

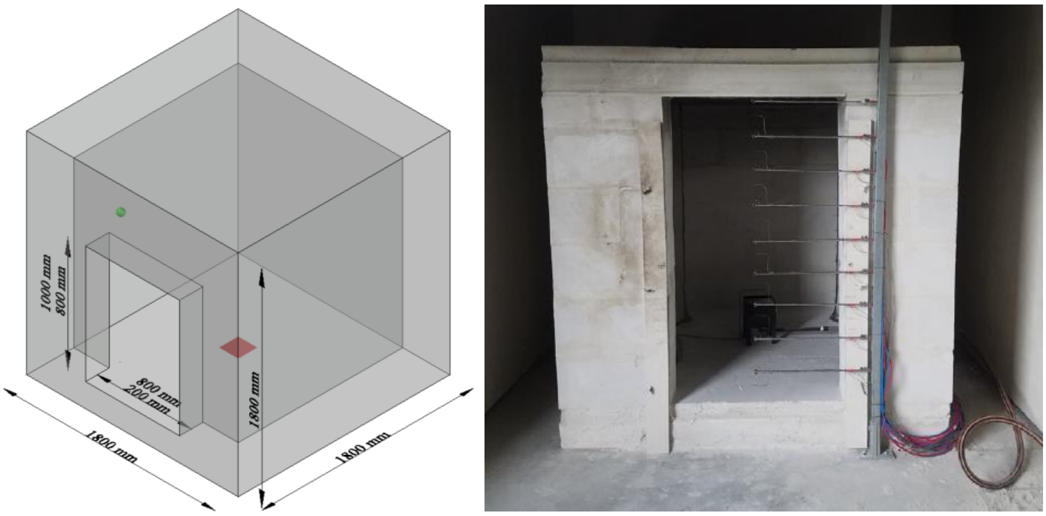

Figure 1. Left) The simulated compartment in FDS. The red square is the fire area, while the location of the thermocouple used for the presented analysis is shown as a green sphere. Right) Real compartment from the experimental campaign [10].

To analyse the wall time of a CFD simulation, the wall time at different timesteps is retrieved from the output file from each simulation, along with the physical seconds in the simulation at the respective timesteps. Based on these data, the goal is to predict the total wall time as soon as possible in the simulation so an early prediction can be given based on limited data. A total of 10 cases are simulated using a computer with a 13th Generation Intel Core i7-13700 processor with a processor speed of 2.1 GHz and 16 cores.

The wall time of the simulations can be determined based on the slope of the wall time as a function of physical seconds, where a steep slope indicates that it takes more time per physical second computed compared to a less steep slope. If the slope of the wall time curve is constant, then the wall time can be estimated accurately early on in the simulation. This paper will investigate this phenomenon for well- and under-ventilated compartments with constant heat release rates.

3. Results

For the five different fire heat release rates and two different compartment ventilation conditions, the heat release rates and temperatures of the various simulations are shown in Figure 2. The temperatures are measured in the front of the compartment at the height of 1 m from the floor, and 0.2 m from either wall in the corner. The location of the thermocouple is shown in Figure 1.

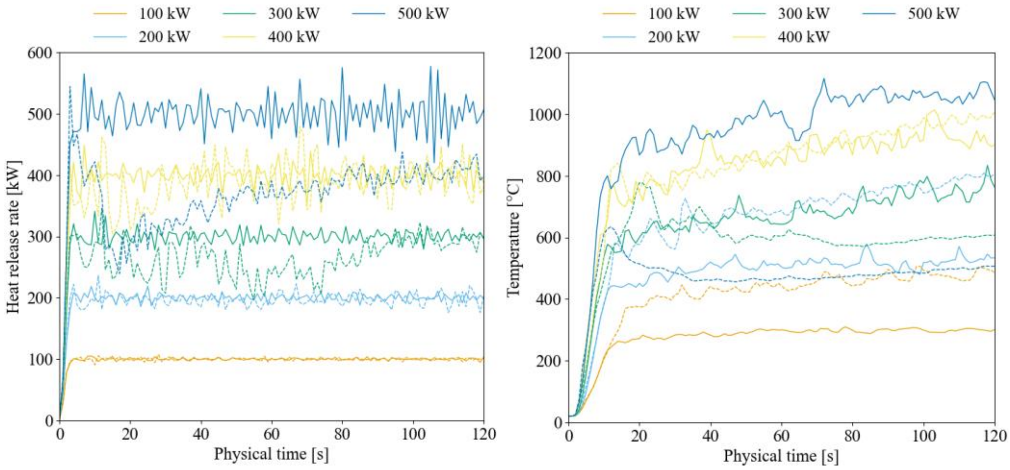

Figure 2. Left: Predicted heat release rate as a function of physical time. Right: Temperature as a function of physical time. The solid lines are for simulations with a ventilation factor of 0.8 $m^{5/2}$ and the dashed lines are for simulations with a ventilation factor of 0.1 $m^{5/2}$.

As shown in Figure 2, the predicted heat release rates vary considerably between the well-ventilated case (ventilation factor of 0.8 $m^{5/2}$) and under-ventilated cases (ventilation factor of 0.1 $m^{5/2}$ and a heat release of more than 200 kW). For nominal heat release rates above 300 kW, the predicted heat release rates in the latter scenarios (smaller opening, ventilation factor of 0.1 $m^{5/2}$) are lower than imposed due to oxygen depletion and flame extinction phenomena. This changes the flow dynamics, as the size of the fire is smaller, hence smaller velocities can be expected. Consequently, the simulation computational time is also expected to reduce.

Figure 3 presents the wall time as a function of the physical time simulated in the CFD simulations for different heat release rates and ventilation factors. The left figure shows the full simulation, while the right figure shows the first 10 seconds of physical time, to highlight the changes in slope during the simulation. The right figure is the subset from the full simulation in the dotted square on the left figure.

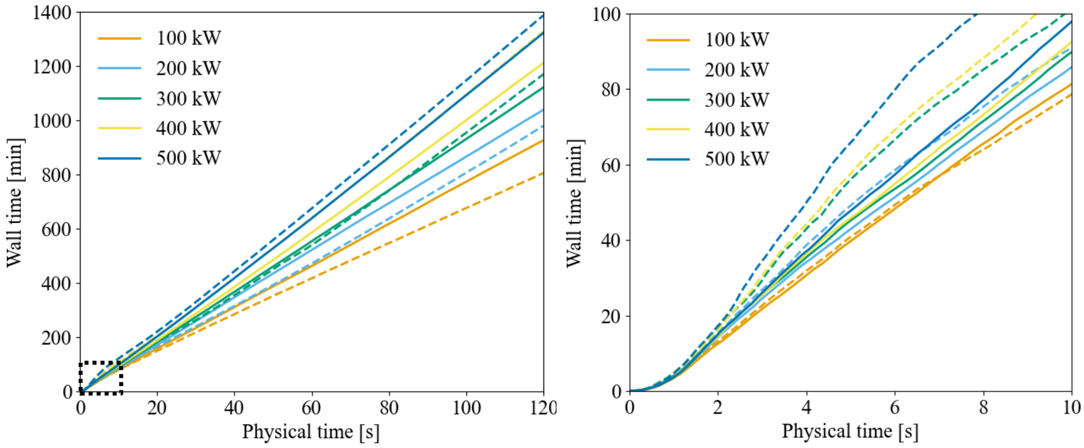

Figure 3. Wall time as a function of physical time (full physical time on the left and initial 10 seconds on the right) in the CFD simulations for different HRRs. The solid line is for a ventilation factor of 0.8 $m^{5/2}$ and the dashed line is for a ventilation factor of 0.1 $m^{5/2}$.

It can be observed that the wall time is highly correlated with the fire HRR. This is to be expected as the velocities are influenced by the size of the fire inside the compartment. A higher HRR implies higher velocities, hence reduced allowed time steps (Eq. (2)). The well-ventilated case can be seen to exhibit a near-constant slope in Figure 3, further re-iterated in Figure 4. This is due to the stable HRR, as seen in Figure 2.

In contrast, the gradient of the wall time for the under-ventilated case is less stable, due to the lower ventilation factor leading to under-ventilated conditions: less oxygen is available, thus reducing the size of the fire and its heat release rate below the prescribed value. From Figure 3 with a ventilation factor of 0.1 $m^{5/2}$, a significant change in slope is exhibited several times during the entire wall time for heat release rates above 300 kW. The slope of the heat release rates changes multiple times for the under-ventilated cases at the same time as the changes in slope of the wall time occur (Figure 2). This is further illustrated in Figure 4, where the slope of the wall time stabilizes only after approximately 30-60 physical seconds for compartments in the under-ventilated regime.

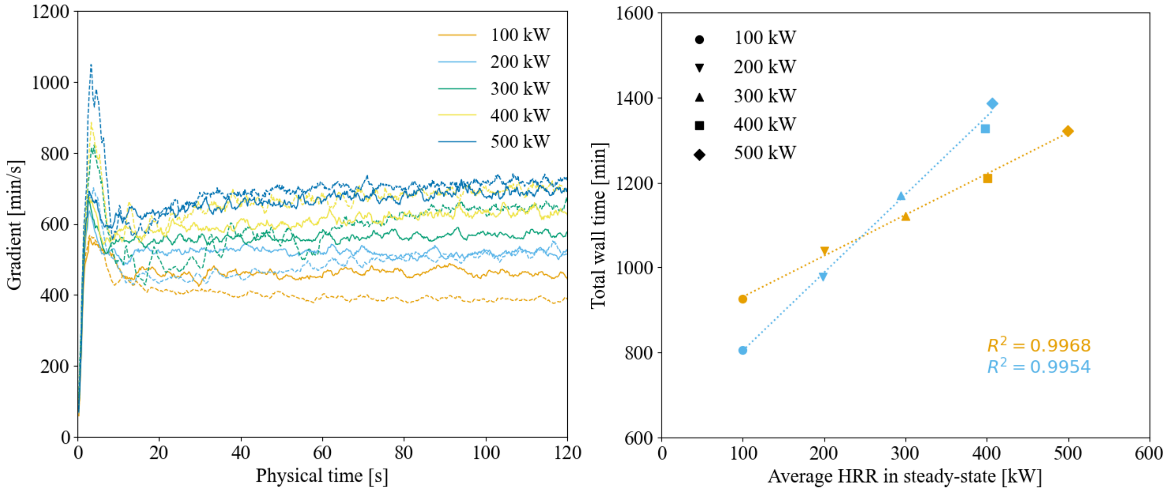

Figure 4. Left: The derivative of the wall time curves as a function of physical time. Solid lines show the derivative for a ventilation factor of 0.8 $m^{5/2}$ and dashed lines show for a ventilation factor of 0.1 $m^{5/2}$. Right: Total wall time as a function of the average HRR at steady state. Orange is for a ventilation factor of 0.8 $m^{5/2}$ and blue is for a ventilation factor of 0.1 $m^{5/2}$.

Based on these simulations, a constant slope is present for the well-ventilated cases and the wall time is proportional to the imposed heat release rate of the simulation (Figure 4, right), making the use of linear extrapolation feasible early on in the simulation. Results of the velocity profile in the opening also show a proportionality between the velocity and the heat release rate (not shown here). For under-ventilated cases, the slope is influenced by the extinction sub-model, which is primarily based on the availability of oxygen in the compartment. More work should be done to investigate if this is due to the total heat release rate or the heat release rate inside the compartment, along with investigating the difference cause for the difference between the imposed heat release rate, and the actual heat release rate. This stabilises later than the well-ventilated cases, with an initial overshoot, followed by a reduced heat release rate compared to the assigned heat release rate in the simulation, and thus a lower slope of the wall time curve. The heat release rate is also less stable than in the well-ventilated. To accurately predict the wall time using linear extrapolation, a constant slope at the stabilised point in the simulation is needed, meaning that the under-ventilated case cannot be predicted as early as the well-ventilated case. From Figure 4, it can be concluded that the total wall-time of a well-ventilated compartments can be estimated early in the simulation, from around 5-10 physical seconds in the simulation. Contrarily, the total wall time of an under-ventilated compartment can be estimated accurately after around 30 physical seconds. Using linear extrapolation at the same point for under-ventilated compartments as the well-ventilated compartments will result in an overestimation of the wall time.

4. Conclusion

The wall time of a CFD simulation is a key factor when allocating computational resources, such that the resource management can be optimised, and an early cost-estimate of the simulation can be performed. This paper investigated the possibility of predicting the total wall time using linear extrapolation, for simulations of different heat release rates and ventilation factors for a cubic compartment. In total, 10 different compartment fire scenarios were investigated with varying fire heat release rates and compartment ventilation factors. A direct proportionality was found between the wall time and the heat release rate, due to the influence on the compartment flow elements.

Based on these results, it can be concluded that accurately predicting the wall time is possible for well-ventilated compartments early in the simulation. On the other hand, the computation of more physical seconds is needed for under-ventilated compartments to accurately predict the total wall time.

For future research, more work should be carried out in estimating the wall time for various physical phenomena that change the heat release rate (e.g., scenarios involving flame spread, oscillatory flames, etc). Particular attention should be paid on the definition of the computational domain to ensure that all combustion products and reactions are computed within the mesh. Different sub-grid scale viscosity models can be investigated as well, to see how the wall time is affected by various sub-models with different numbers of operations required. In contrast, parameters that do not directly influence the velocity of the flow elements are deemed non-influential (such as compartment size and compartment thermo-physical properties).

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