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**Author(s)**  
Yousefian, Sajjad; Gauthier, François; Morán-Guerrero, Amadeo; Richardson, Robert R.; Curran, Henry J.; Quinlan, Nathan J.; Monaghan, Rory F.D.

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A simplified approach to the prediction and analysis of temperature inhomogeneity in rapid compression machines

Sajjad Yousefian,†‡¶ François Gauthier,§ Amadeo Morán-Guerrero,§# Robert R. Richardson,§@@ Henry J. Curran,∥⊥ Nathan J. Quinlan,*§⊥ and Rory F. D. Monaghan †‡¶

Mechanical Engineering, National University of Ireland Galway, Combustion Chemistry Centre, National University of Ireland Galway, Ryan Institute for Environmental, Marine and Energy Research, National University of Ireland Galway, Mechanical Engineering, National University of Ireland Galway., Combustion Chemistry Centre, National University of Ireland Galway., and Ryan Institute for Environmental, Marine and Energy Research, National University of Ireland Galway.

E-mail: nathan.quinlan@nuigalway.ie

Abstract

*To whom correspondence should be addressed
†Mechanical Engineering, National University of Ireland Galway
‡Combustion Chemistry Centre, National University of Ireland Galway
¶Ryan Institute for Environmental, Marine and Energy Research, National University of Ireland Galway
§Mechanical Engineering, National University of Ireland Galway.
∥Combustion Chemistry Centre, National University of Ireland Galway.
⊥Ryan Institute for Environmental, Marine and Energy Research, National University of Ireland Galway.
#Present address: Escuela Técnica Superior de Ingenieros Navales, Universidad Politécnica de Madrid, Spain
@@Present address: Department of Engineering Science, University of Oxford, UK
Substantial progress has been made in understanding and reducing temperature inhomogeneity in rapid compression machines (RCMs) with the help of computational modelling. To date, however, it has not been possible to investigate and map the full range of possible RCM designs, working gases and operating conditions. In this article, we present a framework which simplifies the task of comprehensive and general RCM performance prediction. A set of thermophysical and geometrical parameters have been defined to characterize the design and operating conditions of a general RCM. Dimensional analysis was applied to reduce the number of variables and a sensitivity analysis, based on computational simulations, was used to rank the dimensionless parameters and eliminate unimportant ones. The results of this analysis show that Reynolds number, Prandtl number, aspect ratio, and crevice volume ratio are the most important parameters determining temperature inhomogeneity.

A further set of computational simulations was conducted to predict post-compression temperature inhomogeneity over the full range of RCM design and operating parameters. These results are well represented by a simple power law equation that correlates a dimensionless temperature inhomogeneity parameter (mass-averaged over the main chamber) as a function of post-compression time with just three parameters – Peclet number (the product of Reynolds and Prandtl numbers), aspect ratio, and crevice volume ratio. This equation can serve as a simple and general tool for RCM designers and users who wish to determine optimal configurations that minimise temperature inhomogeneity for combustion experiments.
Nomenclature

\( a \) crevice volume ratio
\( A \) entrance channel inlet height
\( b \) aspect ratio
\( B \) entrance channel outlet height
\( c \) speed of sound
\( c_p \) constant-pressure specific heat
\( C \) Courant number \( C = U \Delta t / \Delta x_0 \)
\( C_v \) constant-volume specific heat
\( D \) diameter
\( d \) entrance channel average height ratio
\( h \) entrance channel average height
\( H \) crevice length
\( k \) thermal conductivity
\( M \) Mach number
\( P \) pressure
\( Pr \) Prandtl number
\( Pe \) Peclet number
\( r \) geometric compression ratio
\( R \) specific gas constant
\( Re \) Reynolds number
\( S \) stroke length
\( T \) temperature
\( t \) time
\( U \) piston velocity
\( V \) volume
\( W \) crevice height
\( X \) dimensionless parameter
\( \alpha \) thermal diffusivity
\( \varepsilon \) normalised temperature difference

Subscripts
\( c \) core
\( cr \) crevice
\( s \) stroke
\( i \) initial
\( w \) wall
\( 0 \) reference
1 Introduction

The objective of this work is to develop a simple and general framework for the computational prediction of temperature inhomogeneity in rapid compression machines (RCMs). The function of an RCM is to provide an environment of uniform, controllable pressure and temperature for the investigation of combustion processes. An RCM consists of a reaction chamber containing a piston which operates in a single rapid stroke to compress the gas mixture under study in an approximately isentropic process. In some RCMs, including the NUI Galway machine, two pistons compress the gas charge symmetrically.

Temperature homogeneity of the compressed gas is a critical attribute of RCMs. Because of the exponential dependence of rate constants on temperature, even minor departures from homogeneity can greatly complicate the interpretation of experimental results. However, it is inevitable that heat transfer to the piston and cylinder (which are typically close to ambient temperature) results in the formation of thermal boundary layers. To some extent, experimental results can be corrected for boundary layer effects by theoretical calculations. A greater problem is caused by the interaction of the piston with the cylinder wall boundary layer. Slow-moving (relative to the cylinder) cool boundary-layer gas flows radially inward along the piston face, and a corner vortex is formed, which transports this gas away from the piston into the core (i.e. the region unaffected by direct boundary-layer heat transfer). The cool gas mixes with compressed core gas in a complex flow field, leading to an inhomogeneous temperature field which cannot be easily predicted. The impact of the corner vortex can be reduced or even eliminated by introducing an annular gap between the piston and cylinder, with a crevice of sufficient volume to contain much of the boundary-layer gas. Various computational fluid dynamics (CFD) studies have been conducted to investigate and optimise the operation of vortex-suppressing crevices.

Thus, major advances have been achieved in understanding and reducing temperature inhomogeneity in RCMs. Until recently, however, each investigation of RCM heat transfer and fluid dynamics has necessarily been restricted to a specific machine at a restricted range
of operating conditions. No general rules are available for the design and operation of RCMs to optimise homogeneity. The reason for this is the large number of variables which may influence the flow and temperature field, including gas thermophysical properties and the kinematic and geometric parameters of the RCM. For example, Mittal et al.\textsuperscript{7} conducted a programme of simulations which yielded data for a temperature inhomogeneity measure as a function of stroke length, compressed gas pressure and Argon-Nitrogen mixture fraction in a particular RCM. This is probably the most comprehensive RCM temperature inhomogeneity performance map to date. However, as we will argue in Section 2, RCM performance depends on as many as 13 variables characterising machine dimensions, operating conditions and gas thermophysical properties. It is impractical to characterise RCM performance completely as a function of all these variables, by a direct campaign of either computation or experiments.

The objective of the present work is to enable the prediction of temperature inhomogeneity by computational methods for the most general RCM design and operating conditions. We take two approaches to systematically reduce the cost of such an investigation. The first approach is a dimensional analysis to recast the problem and characterize performance of RCM in terms of thermophysical and geometrical dimensionless parameters in place of the usual physical variables. This is an exact mathematical operation involving no approximations. In effect, it removes redundant information from the specification of the problem. Dimensional analysis has the added advantage of permitting results to be formulated independently of scale, so that data can be generalised to a wide range of systems. The second stage is a set of preliminary computations to investigate the sensitivity of RCM operation to each dimensionless variable, with a view to eliminating variables that have relatively small effects.

Based on this approach, a set of CFD simulations was carried out which predict temperature inhomogeneity for a general RCM across a wide range of conditions. These results are used to correlate a dimensionless temperature inhomogeneity parameter as a function of RCM design and operating parameters.
A dimensional analysis of RCM temperature inhomogeneity is presented in section 2. The computational method is described in section 3. Some representative CFD results are presented in detail in section 4.1. Results of the sensitivity analysis are presented in section 4.2. The subsequent parametric CFD study, based on variables identified by dimensional analysis and sensitivity study, are shown in section 4.3 with the resulting correlation for temperature inhomogeneity.

2 Dimensional analysis

The purpose of this dimensional analysis is to identify the minimum set of variables that can fully define the RCM and its operating condition. First, the problem must be formulated mathematically. For an RCM with a simple cylinder and a flat piston, the design and operating conditions are fully specified by stroke length $S$, main chamber diameter $D$, average piston velocity $U$, initial pressure $P_i$, initial temperature $T_i$, geometric compression ratio $r$, gas constant $R$, specific heat ratio $\gamma$, thermal conductivity $k$, and dynamic viscosity $\mu$. This is not the only valid choice for this set of parameters; for example, $R$ could be replaced with $c_p$. The state of the RCM also depends on time $t$.

Additional parameters are required to define the geometry of a piston head crevice. The geometry of the NUI Galway RCM is shown in Figure 1 with a generic crevice. Previous research suggests that crevice volume $V_{cr}$ is the most important property of the crevice in determining its capability to suppress vortices. We therefore include this parameter. The annular entrance channel from the main chamber to the crevice may affect performance, and therefore we also include the average radial width of the channel, $h = (A + B)/2$, where $A$ and $B$ are defined in Fig. 1.

The temperature-dependent gas properties $\gamma$, $k$, and $\mu$ vary throughout both the compression and constant-volume phases of an RCM experiment. To evaluate them, a reference mid-compression condition is defined. This is the idealised condition reached by isentropic
compression with constant value of $\gamma$ denoted as $\gamma_i$, starting from the initial pressure, with a pressure ratio equal to half the overall isentropic pressure ratio $r_p = r^\gamma$. This midpoint pressure $\hat{P}$ is $P_i r^{\gamma_i}/2$ and the midpoint temperature $\hat{T}$ is $T_i r^{(\gamma_i-1)/2(r_i-\gamma_i)}$. Reference property values $\hat{\gamma}$, $\hat{\mu}$ and $\hat{k}$ are evaluated at this midpoint state. Similarly, the piston velocity is a function of time in an RCM experiment, and is represented by the average velocity $\bar{U} = S/t_c$ from start to stop of the compression stroke.

To quantify the performance of the RCM, we define a local dimensionless temperature difference $\varepsilon$ as

$$\varepsilon(r, z, t) = \frac{T_c(t) - T(r, z, t)}{T_c(t) - T_w}$$

where $(r, z)$ are cylindrical polar coordinates, $T_c(t)$ is the core temperature, defined as the instantaneous maximum temperature in the RCM main chamber, and $T_w$ is the wall temperature. For simulations presented later in this work, wall temperature is equal to the initial gas temperature. A useful temperature inhomogeneity parameter can then be defined as the spatial average of $\varepsilon$ over the whole of the main chamber:

$$\bar{\varepsilon}(t) = \frac{T_c(t) - \bar{T}(t)}{T_c(t) - T_w}$$
where $\bar{T}(t)$ is the mass-average temperature in the main chamber (excluding the crevice, if there is one). A value of $\bar{\epsilon}$ close to 1 implies that $\bar{T} \simeq T_w$, indicating that the bulk gas temperature is dominated by wall heat transfer, while $\bar{\epsilon} \simeq 0$ implies that gas temperature everywhere is close to the core temperature, and thus wall effects are small. This is similar to the “% influence” defined by Mittal et al.\textsuperscript{7} In the present work, however, a different normalisation is employed, giving special meaning to $\bar{\epsilon} = 0$, and $\bar{\epsilon}$ is based on the whole of the main chamber, whereas Mittal et al. excluded the calculated thermal boundary layer.

Thus, the parameter $\bar{\epsilon}$ (or any measure of the RCM’s thermomechanical performance) is determined by the design and operating parameters according to an as yet unknown relationship of the form

$$\bar{\epsilon} = \bar{\epsilon}(S, \bar{U}, P_i, T_i, r, D, V_{cr}, h, R, \dot{\gamma}, \dot{k}, \dot{\mu}, t)$$

Thus, there are 13 independent variables which characterise the RCM and determine the one dependent variable, $\bar{\epsilon}$. These 13 quantities have 4 fundamental dimensions, mass, length, time and temperature. According to the Buckingham Pi theorem, this can be reduced to a relationship involving $(14 - 4 = 10)$ dimensionless parameters.

Several equally valid choices are possible for a set of 10 parameters. However, some choices are more useful than others in enabling various physical effects to be distinguished clearly. The chosen set includes temperature inhomogeneity $\bar{\epsilon}$, geometric compression ratio $r$, and specific heat ratio $\dot{\gamma}$, which are already dimensionless in the original set of variables. Time as non-dimensionalised as

$$t^* = \frac{t}{S/\bar{U}}$$

where $t = 0$ is defined as the end of compression and $S/\bar{U}$ is the time taken for the compression stroke, so that compression begins at $t = -S/\bar{U}$. The chosen parameter set also includes the well-known Reynolds, Mach and Prandtl numbers, $Re_S$, $M$, and $Pr$, all based on reference mid-compression conditions. They can be expressed as follows in terms of the
original variables of Eq. (3):

\[
Re_S = \frac{\hat{\rho} \bar{U}_S}{\hat{\mu}} = \frac{r P_i}{2 \hat{\gamma}_i R T_i} \frac{\bar{U} S}{\hat{\mu}}
\]

(5)

\[
M = \frac{\bar{U}}{\bar{c}} = \frac{\bar{U}}{\sqrt{\hat{\gamma} R T_i}} = \frac{2^{(\gamma_i - 1)/2\gamma_i} \bar{U}}{r^{(\gamma_i - 1)/2} \sqrt{\hat{\gamma} R T_i}}
\]

(6)

\[
Pr = \frac{\hat{c}_p \hat{\mu}}{\hat{k}}
\]

(7)

Reynolds number is based on stroke length, since it is the stroke that governs the growth of the boundary layer and the formation of the roll-up vortex during compression. The three remaining dimensionless parameters characterise the geometry, and were constructed by grouping physically related parameters. Since the main function of the crevice is to accommodate the boundary layer from the swept volume, crevice volume \( V_{cr} \) is normalised to swept volume to give

\[
a = \frac{4V_{cr}}{\pi D^2 S}
\]

(8)

The aspect ratio of the swept volume is defined as

\[
b = \frac{D}{2S}
\]

(9)

normalising to stroke length rather than final clearance or any other length, again because of the dependency of boundary layer formation on stroke length. Main chamber radius \( D/2 \) determines how much space there is for the gas to flow from the corner towards the centreline. Therefore, entrance channel average height ratio is defined as

\[
d = \frac{2h}{D}
\]

(10)

The resulting dimensionless functional relationship is

\[
\bar{\varepsilon} = \bar{\varepsilon}(Re_S, Pr, M, \hat{\gamma}, r, b, a, d, t^*)
\]

(11)
which is precisely equivalent to Eq. (3).

Dimensional analysis has shown that the performance of the RCM with flexible geometry is truly dependent on only 9 independent dimensionless parameters instead of 13 independent variables as shown in equation 3. The approach adopted in this work is to characterise the performance of the RCM by modelling it computationally at a matrix of operating conditions sampled across the possible range. Although dimensional analysis reduces the parameter space from 13 dimensions to 9, the computational effort required to completely map this space is still prohibitive. Therefore, a sensitivity analysis was conducted to limit computational cost, as described in section 4.2.

3 CFD modeling approach

3.1 RCM geometry and computational domain

The parametric internal dimensions of the generic RCM are shown in Fig. 1, with the NUI Galway RCM for illustration. The RCM is shown with a creviced piston head in its initial and final position. In the reference configuration, the internal diameter is \( D = 38.2 \) mm, stroke length of each piston is \( S = 172 \) mm, piston-to-midplane distance \( L_f = 16.5 \) mm (half of the final clearance length), crevice length \( W = 2.7 \) mm, crevice height \( H = 8.1 \) mm, entrance channel inlet height \( A = 0.412 \) mm, and entrance channel outlet height \( B = 0.150 \) mm. The average channel height is \( h = 0.281 \) mm. The piston displacement history is prescribed as a polynomial fit to experimentally measured piston position data, as shown in Fig. 2. To vary piston velocity, this function is simply scaled.
Figure 2: Experimentally measured displacement of the piston (dots), with the polynomial fit prescribed in the computational model (solid curve).

3.2 Computational method

The flow is assumed symmetric about the cylinder axis and the mid plane, and free of swirl. This facilitates a 2D axisymmetric model bounded by the cylinder, the piston, the centreline axis of symmetry, and the midplane, as shown in Fig. 1. Würmel et al.\textsuperscript{2} used a symmetrical boundary condition in their simulation for the same configurations. The piston and cylinder surfaces are modelled as isothermal no-slip walls at a temperature equal to the initial gas temperature. The flow was simulated using ANSYS Fluent v16.0 with the PISO algorithm for pressure-velocity coupling, PRESTO pressure gradient evaluation, and second order upwind scheme for density, momentum and energy. Twenty iterations were run per time step and globally scaled residuals (normalised to global sums) fell below $10^{-4}$ for continuity, $10^{-6}$ for momentum, and $10^{-10}$ for energy. Temperature-dependent gas thermophysical properties are evaluated by polynomial fits to NIST data.\textsuperscript{8} Simulations were carried out on Fionn, an Intel Xeon E5-based cluster at the Irish Centre for High-End Computing. The total computational cost was 32,400 CPU-hours for the 90 simulations described in this work.

Tabaczynski et al.\textsuperscript{3} found that incompressible, isothermal corner flow is laminar for Reynolds number, based on stroke length and piston velocity, up to 12,500. However, no clear
criterion exists for laminar-turbulent transition in the more complex compressible flow of an RCM. Previous CFD simulations for RCMs have been based on a laminar model, RANS turbulence models, and large eddy simulation (LES). Mittal and Sung observed that laminar computations yield closer agreement with planar laser-induced fluorescence (PLIF) experimental temperature measurements than a RANS turbulence model, and Würmel and Simmie found that the use of a $k - \varepsilon$ turbulence model has very small effects on simulations of the NUI Galway RCM. Recent work by Ihme and Grogan et al. focused on ignition regimes and interaction of turbulence and chemistry, using Reynolds and Damkohler scaling in a spatially homogeneous model. Ihme emphasized that the relative contributions of different mechanisms of turbulence in RCM have so far not been experimentally quantified and are most likely dependent on facility design and operation conditions. Banaeizadeh simulated the Michigan State University (MSU) RCM with LES, but found that results disagreed with experimental data in case of a flat piston.

Thus, computational modelling of turbulent flow in an RCM remains an open challenge, due in part to the low Reynolds number (in terms of turbulent flows) and the coexistence of laminar and turbulent regions. Current creviced piston head configurations are based on a laminar model. Since there is no experimental validation to confirm that any specific turbulence model for CFD simulation of RCM is more accurate than a laminar model, a turbulence model is not used in the present work.

### 3.3 Computational grid

As the piston moves, the mesh must conform to the decreasing volume of the domain. This is managed using the dynamic mesh layering scheme of ANSYS Fluent. The mesh as a whole translates with the piston, except for the layer of cells adjacent to the symmetry plane, which are reduced in axial length. When the length of these cells has decreased by a specified ratio, they are merged with the full-size cells in the next layer. This method allows the mesh in the area of most complex flow (near the piston) to remain constant, and results in faster
computation due to the decrease in number of cells as compression proceeds. The initial gas volume is discretised with a block-structured mesh of 39,019 quadrilateral cells, refined near walls and in the crevice channel to enhance resolution of the thermal and momentum boundary layers. The computational grid and boundary conditions is shown in Fig. 3 at the end of compression with an enlarged view of entrance channel, where the mesh is finest. The time step $\Delta t$ is 4 $\mu$s. The Courant number based on local velocity and cell length was less than 1 everywhere in the main chamber at all times. The smallest axial mesh cell length is 0.020 mm and the smallest radial mesh cell length is 0.006 mm.

Figure 3: Computational mesh and boundary conditions at the end of compression, with an enlarged view of the entrance channel region ($L_f = 16.5$ mm).

This spatial and temporal resolution are consistent with or better than previous work on RCM models. Würmel and Simmie$^2$ employed a mesh of 9,000 cells ranging in length from 0.1 to 0.7 mm with a timestep of 8 $\mu$s. Mittal and Sung$^6$ used 14,000 cells with a timestep of 56 $\mu$s and Mittal et al.$^7$,$^{10}$ used a timestep of 42 $\mu$s.
4 Computational Results

4.1 Reference condition

The results of CFD simulations for the NUI Galway RCM containing nitrogen at initial temperature 313 K and initial pressures of 50 kPa and 100 kPa are shown in Fig. 4. Temperature distribution in the main chamber and crevice, and velocity distribution in the main chamber, are presented at times from 0 to 200 ms post-compression. Throughout this work, time $t = 0$ is defined as the end of the compression stroke. The corresponding dimensionless parameters are $r = 11.42$, $\dot{\gamma} = 1.37$, $Re_S = 2.07 \times 10^5$, $Ma = 0.0197$, $Pr = 0.73$, $a = 0.0105$, $b = 0.111$, and $d = 0.0147$. This case, with initial pressure of 50 kPa, is defined as the reference operating condition for the present study.

It is seen from Fig. 4 that with $P_i = 100$ kPa, there is only one vortex on the piston face (for one quarter of the computational domain), and this vortex grows with time after compression. In contrast, for $P_i = 50$ kPa, the vortex shown in Fig. 4 is larger even at the end of compression. Later, two vortices develop with higher velocity magnitude, mixing cooler boundary layer gas into the core. It is therefore computationally demonstrated that the roll-up vortex is pressure-dependent. This result is consistent with CFD results of Mittal et al.\textsuperscript{7} and PLIF measurements of the temperature field reported by Mittal and Sung.\textsuperscript{6} The well-known mechanisms of RCM temperature inhomogeneity\textsuperscript{2–7} can be observed.
4.2 Sensitivity to dimensionless parameters

A sensitivity study was conducted to assess the relative magnitude of effects of the dimensionless parameters. The operating condition was perturbed from the reference case (defined in section 4.1) by adjusting each dimensionless parameter in turn while holding the others constant. The resulting change in the temperature inhomogeneity parameter $\bar{\varepsilon}$ provides a measure of sensitivity to the perturbed parameter. Dimensionless time is not considered,
since inhomogeneity is expected to be highly time-dependent (see, for example, Fig. 4). For analysis of sensitivity to all other variables, $\bar{\varepsilon}$ is sampled at 30 ms post-compression. The value of $\bar{\varepsilon}$ in the reference case is denoted $\bar{\varepsilon}_0$, and the quantity $(\bar{\varepsilon} - \bar{\varepsilon}_0)/\bar{\varepsilon}_0$ is a fractional change in $\bar{\varepsilon}$ resulting from a perturbation of one parameter.

To enable a comparison of sensitivity to different parameters, the magnitude of the perturbations should be chosen in a consistent manner. It would be meaningless to perturb each parameter by the same fraction. For example, it is straightforward to raise the Reynolds number by 50% or more by choosing a denser gas, but impossible to raise $\gamma$ by 50% from 1.4. Instead, each dimensionless parameter is perturbed by 10% of its possible range. This possible range is based on estimates of the minimum and maximum values of each parameter that can practically be attained in an RCM. Where there is uncertainty as to these limits, the estimate errs towards a larger range to enable a comprehensive characteristic map for RCM operation. Argon and nitrogen are normally used as diluent gases. We also consider helium, which enables low Reynolds and Mach numbers, and helium mixtures, which enable the experiment to reach very low $Pr$. Minimum and maximum values for geometrical dimensionless parameters are defined using data reported by Goldsborough$^{16}$ and Mittal$^{17}$ for various RCMs.

The resulting ranges for the dimensionless parameters are shown in Table 1.

Table 1: Minimum and maximum range of dimensionless parameters for sensitivity study.

<table>
<thead>
<tr>
<th>Dimensionless parameter</th>
<th>Minimum</th>
<th>Maximum</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Pr$</td>
<td>0.15</td>
<td>0.85</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>1.3</td>
<td>1.7</td>
</tr>
<tr>
<td>$Re_S$</td>
<td>$2 \times 10^3$</td>
<td>$8 \times 10^5$</td>
</tr>
<tr>
<td>$M$</td>
<td>0.004</td>
<td>0.04</td>
</tr>
<tr>
<td>$r$</td>
<td>8</td>
<td>40</td>
</tr>
<tr>
<td>$a$</td>
<td>0.004</td>
<td>0.07</td>
</tr>
<tr>
<td>$b$</td>
<td>0.04</td>
<td>0.2</td>
</tr>
<tr>
<td>$h$</td>
<td>0.005</td>
<td>0.03</td>
</tr>
</tbody>
</table>

Based on these ranges and reference values, the 10% perturbed values are defined by Eq.
An important step for sensitivity analysis is the determination of dimensional thermo-physical and geometrical variables for each perturbation of the dimensionless parameters. These dimensional values, required for the computational simulations, can be recovered from the dimensionless parameters using Eqs. (13–20).

\[ \hat{k} = (S\hat{T}^{1/2})M\hat{\gamma}^{3/2}(\hat{\gamma} - 1)^{-1}Re_S^{-1}Pr^{-1} \]  
(13)

\[ \hat{\mu} = (S\hat{T}^{1/2}R^{1/2})M\hat{\gamma}^{-1/2}Re_S^{-1} \]  
(14)

\[ \hat{U} = (\hat{T}^{1/2}R^{1/2})M\hat{\gamma}^{1/2} \]  
(15)

\[ \hat{c}_p = R\hat{\gamma}(\hat{\gamma} - 1)^{-1} \]  
(16)

\[ L_f = S(r - 1)^{-1} \]  
(17)

\[ V_{cr} = \pi S^3 b^2 a \]  
(18)

\[ h = Sdb \]  
(19)

\[ D = 2Sb \]  
(20)

This system of equations enables desired values of 9 dimensionless numbers to be set by varying the 8 dimensional parameters on the left-hand side, which are direct inputs to the computational simulation. (One of the dimensionless numbers, \( \hat{\gamma} \), is itself a direct input.)

For example, to perturb \( Pr \), the value of thermal conductivity \( \hat{k} \) should be altered, since \( Pr \) appears only in Eq. (13) above. To perturb \( Re_S \) alone, \( \hat{\mu} \) is adjusted according to Eq. (14), but \( \hat{k} \) is also adjusted according to Eq. (13) (which includes \( Re_S \) on the right-hand side) to avoid an unwanted perturbation of \( Pr = \hat{\mu}\hat{c}_p/\hat{k} \). Alternative formulations could be derived by choosing a different set of 8 dimensional parameters, but according to the Buckingham Pi Theorem, all formulations are equivalent when results are non-dimensionalised.

Each perturbed condition was simulated computationally. Results of the sensitivity study
for 30 ms after the end of compression are shown in Fig. 5. Temperature inhomogeneity $\bar{\varepsilon}$ decreases by approximately 16.7% for a perturbation of $Re_S$ by 10% of its range, 10.3% for a corresponding perturbation of $b$, 7.2% for a perturbation of $a$, and 4.6% for a perturbation of $Pr$. Changes in $\bar{\varepsilon}$ due to $\gamma$, $r$, $d$, and $M$, are all less than 2%. These results show that Reynolds number, aspect ratio, crevice volume ratio, and Prandtl number are significantly more important than the remaining parameters in determining temperature inhomogeneity.

![Diagram showing fractional change in temperature inhomogeneity parameter $(\bar{\varepsilon} - \bar{\varepsilon}_0)/\bar{\varepsilon}_0$ resulting from perturbation of each dimensionless parameter by 10% of its range at 30 ms after the end of compression.]

**Figure 5:** Fractional change in temperature inhomogeneity parameter $(\bar{\varepsilon} - \bar{\varepsilon}_0)/\bar{\varepsilon}_0$ resulting from perturbation of each dimensionless parameter by 10% of its range at 30 ms after the end of compression.

### 4.3 Correlation of temperature inhomogeneity

Based on the results of the sensitivity analysis presented above, a parametric study was conducted to investigate the effect of the four most important parameters – Reynolds number, Prandtl number, aspect ratio, and crevice volume ratio – on temperature inhomogeneity. A CFD simulation was completed for all possible combination of the minimum, maximum and geometric average values of each parameter according to table 2.
Table 2: Minimum, geometric average and maximum values of each dimensionless parameter used in the parametric study.

<table>
<thead>
<tr>
<th>Dimensionless parameter</th>
<th>Minimum</th>
<th>Average</th>
<th>Maximum</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Pr$</td>
<td>0.150</td>
<td>0.357</td>
<td>0.850</td>
</tr>
<tr>
<td>$Re_S$</td>
<td>$2 \times 10^3$</td>
<td>$40 \times 10^3$</td>
<td>$800 \times 10^3$</td>
</tr>
<tr>
<td>$a$</td>
<td>0.004</td>
<td>0.009</td>
<td>0.020</td>
</tr>
<tr>
<td>$b$</td>
<td>0.070</td>
<td>0.118</td>
<td>0.200</td>
</tr>
</tbody>
</table>

This entails $3^4 = 81$ cases, each one simulated up to dimensionless time $t^* = 12$, which corresponds to 200 ms post-compression in the NUI Galway machine. A full time-history of the temperature inhomogeneity parameter $\bar{\varepsilon}$ was recorded for every case. The resulting dataset can be represented by a correlation

$$\bar{\varepsilon} = \bar{\varepsilon}(Re, Pr, a, b, t^*) \quad (21)$$

To determine a simple form for this correlation, an exponential function is used to approximate the growth of temperature inhomogeneity during long post-compression times.

$$\bar{\varepsilon}_p(Re, Pr, a, b, t^*) = \bar{\varepsilon}_\infty - (\bar{\varepsilon}_\infty - \bar{\varepsilon}_0) e^{-\beta t^*} \quad (22)$$

In the above equation, subscript $p$ denotes prediction based on correlation of the computational results. Temperature inhomogeneity parameters $\bar{\varepsilon}_0$ and $\bar{\varepsilon}_\infty$ are predicted values at the end of compression ($t^* = 0$) and the asymptotic final state ($t^* \to \infty$), respectively. The dimensionless $\beta$ characterises the post-compression rate of growth of inhomogeneity. $\bar{\varepsilon}_\infty$, $\bar{\varepsilon}_0$, and $\beta$ depend on Reynolds number, Prandtl number, aspect ratio, and crevice volume ratio, but are independent of time, by definition (these dependencies are not shown in Eq. 22, for conciseness). By minimising least-squares error, the following power-law correlations were
identified.

\[ \beta = 3.30 Re^{-0.32} Pr^{-0.26} a^{-0.08} b^{-0.40} \]  \hspace{1cm} (23)

\[ \bar{\varepsilon}_{0 p} = 1.56 Re^{-0.47} Pr^{-0.44} a^{-0.07} b^{-0.63} \]  \hspace{1cm} (24)

\[ \bar{\varepsilon}_{\infty p} = 1.65 Re^{-0.22} Pr^{-0.22} b^{-0.33} \]  \hspace{1cm} (25)

To illustrate the quality of the exponential model for time-dependence, the computed temperature inhomogeneity parameter \( \bar{\varepsilon}_c \) and predicted \( \bar{\varepsilon}_p \) are plotted in Fig. 6 for some representative cases. Across the range of cases simulated, the exponential fit provides an acceptable representation of the computational results.

\[ \bar{\varepsilon}_p = f(Re, Pr, a, b) \]

Figure 6: Computed and predicted temperature inhomogeneity parameters \( \bar{\varepsilon}_c \) and \( \bar{\varepsilon}_p \) respectively, as functions of dimensionless post-compression time \( t^* \) for different combinations of Prandtl number \( Pr \), Reynolds number \( Re \), crevice volume ratio \( a \), and aspect ratio \( a \).

The temperature inhomogeneity \( \bar{\varepsilon}_p \) predicted by the above correlation is plotted in Fig. 7, in comparison with the values \( \bar{\varepsilon}_c \) directly computed in CFD simulations, for dimensionless times \( t^* = 0 \), \( t^* = 6 \), and \( t^* = 12 \). Instantaneous distributions of dimensionless temperature difference \( \varepsilon(r, \theta, z, t) \) are also shown for a sample of representative cases, including the
reference case, at the end of compression. There is close agreement between predicted and
computed values for the temperature inhomogeneity parameter $\bar{\varepsilon}$.

Figure 7: Predicted temperature inhomogeneity parameter $\bar{\varepsilon}_p$ as a function of Reynolds
number, Prandtl number, crevice volume ratio, and aspect ratio, compared with computed
temperature inhomogeneity parameter $\bar{\varepsilon}_c$ for post-compression dimensionless times $t^* = 0,$
$t^* = 6,$ and $t^* = 12$. The solid line denotes $\bar{\varepsilon}_p = \bar{\varepsilon}_c$ and dashed lines correspond to $\pm 20\%$.

The close similarity of the exponents of $Re_S$ and $Pr$ in Eqs. (23–25) suggests that the
data can be correlated as a function of the single parameter $Re_S Pr$, known as the Peclet
number $Pe$, which quantifies the ratio of convective to conductive heat transfer. This results
in new coefficients as follows.

$$\beta = 3.08 Pe^{-0.32} a^{-0.08} b^{-0.40}$$  \hspace{1cm} (26)

$$\bar{\varepsilon}_0p = 1.49 Pe^{-0.47} a^{-0.07} b^{-0.63}$$  \hspace{1cm} (27)

$$\bar{\varepsilon}_\infty p = 1.66 Pe^{-0.22} b^{-0.33}$$  \hspace{1cm} (28)

As shown in Fig. 8, the predicted results again display close agreement with the 81 com-
putational results. Thus, to a good approximation, temperature inhomogeneity depends on
only Peclet number $Pe$, crevice volume ratio $a$, and aspect ratio $b$, which characterize the RCM gas properties and configuration.

![Figure 8: Predicted temperature inhomogeneity parameter $\bar{\varepsilon}_p$ as a function of Reynolds number, Prandtl number, crevice volume ratio and aspect ratio, compared with computed temperature inhomogeneity parameter $\bar{\varepsilon}_c$ for dimensionless post-compression times $t^* = 0$, $t^* = 6$, and $t^* = 12$. The solid line denotes $\bar{\varepsilon}_p = \bar{\varepsilon}_c$ and dashed lines correspond to $\pm 20\%$.]

The distinct effects of $Pe$, $a$ and $b$ on temperature inhomogeneity parameter are differentiated in Figs. 9, 10 and 11 for dimensionless post-compression times of $t^* = 0, 6, 12$ respectively (corresponding to 0 ms, 100 ms and 200 ms after compression in the NUI Galway RCM). Since $Pe$ now replaces $Re$ and $Pr$, only 27 data points are shown instead of 81 data points. Similar trends can be observed at all times. Inhomogeneity parameter $\bar{\varepsilon}$ increases with decreasing $Pe$, $a$ and $b$. Peclet number has by far the largest influence, followed by aspect ratio $b$ and crevice volume ratio $a$. This multivariable analysis confirms the results of the sensitivity analysis, which was based on perturbations of a single variable.
Figure 9: The effect of Peclet number $Pe$, crevice volume ratio $a$, and aspect ratio $b$ on temperature inhomogeneity parameter $\bar{\varepsilon}$ values for $t^* = 0$. $Pe$, $a$ and $b$ are coded by symbol shape, colour and size, respectively. The solid line denotes $\bar{\varepsilon}_p = \bar{\varepsilon}_c$ and dashed lines correspond to $\pm 20\%$.

Figure 10: The effect of Peclet number $Pe$, crevice volume ratio $a$, and aspect ratio $b$ on temperature inhomogeneity parameter $\bar{\varepsilon}$ values for $t^* = 6$. $Pe$, $a$ and $b$ are coded by symbol shape, colour and size, respectively. The solid line denotes $\bar{\varepsilon}_p = \bar{\varepsilon}_c$ and dashed lines correspond to $\pm 20\%$. 

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Figure 11: The effect of Peclet number $Pe$, crevice volume ratio $a$, and aspect ratio $b$ on temperature inhomogeneity parameter $\bar{\varepsilon}$ values for $t^* = 12$. $Pe$, $a$ and $b$ are coded by symbol shape, colour and size, respectively. The solid line denotes $\bar{\varepsilon}_p = \bar{\varepsilon}_c$ and dashed lines correspond to $\pm 20\%$.

5 Discussion

For a wide range of geometrical parameters and thermophysical operating conditions, dimensional analysis shows that heat transfer and fluid dynamics are dependent on 8 dimensionless parameters (plus time), instead of 12 gas and machine properties. Various choices of the 8 parameters are possible; we select Reynolds number $Re_S$, Prandtl number $Pr$, Mach number $M$, specific heat ratio $\gamma$, geometric compression ratio $r$, aspect ratio $b$, crevice volume ratio $a$, and entrance channel average height ratio $d$.

In a series of preliminary computational models for sensitivity analysis, it was shown that four parameters (Reynolds, Prandtl numbers, aspect ratio, and volume crevice ratio) have significantly greater effects than the others on temperature inhomogeneity. These effects are quantified in terms of the sensitivity of temperature inhomogeneity to each parameter over
the practically possible range of that parameter.

Based on the results of the dimensional analysis and sensitivity analysis, a generic RCM was simulated over compression and 200 ms post-compression (i.e. a post-compression period 12 times longer than compression time) over a range of Reynolds, Prandtl numbers, aspect ratio, and crevice volume ratio in order to map temperature inhomogeneity over the full operating range of the machine. Results can be predicted with a correlation of the form \( \bar{\epsilon}_p(Re, Pr, a, b, t^*) = \bar{\epsilon}_{\infty p} - (\bar{\epsilon}_{\infty p} - \bar{\epsilon}_{0p})e^{-\beta t^*}, \) where \( t^* \) is dimensionless time for post-compression and \( \bar{\epsilon}_{\infty p}, \bar{\epsilon}_{0p}, \) and \( \beta \) are power-law functions of Reynolds number, Prandtl number, aspect ratio, and crevice volume ratio. The correlation can be further simplified, without loss of accuracy, by introducing Peclet number \( Pe = ReSPr = Us\rho cp/k, \) which represents the order of magnitude of the ratio of energy fluxes due to convective transport and diffusion (conduction). It describes the balance between fundamental physical mechanisms of heat transfer in the RCM. Alternatively, \( Pe \) can be rewritten as \( US/\alpha, \) offering another interpretation: the primary gas property that affects temperature (in)homogeneity is the thermal diffusivity, \( \alpha. \) The importance of \( \alpha \) has previously been highlighted in the work of Mittal et al.\(^7\)

The volumetric compression ratio (or the pressure ratio, which could appear in an equally valid alternative formulation of the results) is absent from the final correlations. This may appear to conflict with previous results (Mittal et al.\(^7\) and Fig. 4) that show a strong effect of final pressure on temperature inhomogeneity. However, there is no contradiction. In the previous, pressure ratio affects temperature inhomogeneity but does so through its effect on density, and hence thermal diffusivity and (most fundamentally) Peclet number. The pressure is important not as a thermodynamic property, but as an indirect influence on transport processes. In the present computational study, compression ratio has been varied while holding the Peclet number constant, isolating the effects of each variable. The effect of pressure ratio has been compounded with Peclet number effects in previous work.

The absence of Mach number \( M \) from the list of important variables is to be expected
within the low range of possible values ($0.004 \lesssim M \lesssim 0.04$). For piston Mach numbers close to 1 (extremely high piston speed), the duration of piston travel would be of the same order as the transit time of the compression or shock waves created by its acceleration. Significant spatial inhomogeneity would result directly from the compression process itself. At the very low Mach numbers typical of RCMs, however, many transits of acoustic compression waves occur while the piston is in motion, enabling the temperature field to remain spatially uniform (in the absence of wall heat transfer).

Mittal et al.\textsuperscript{7} examined the effect of several parameters on vortex formation and temperature inhomogeneity in an RCM with a creviced piston. They observed that higher absolute pressure results in a smaller vortex and a more homogeneous temperature field. This is consistent with the findings of the present dimensionless framework and CFD simulations of the reference case, since high pressure results in higher density and hence higher Peclet number. Mittal et al.\textsuperscript{7} also reported that vortex formation and temperature inhomogeneity decreased with increasing clearance length (i.e. increasing final volume) for constant stroke length and approximately constant final conditions. However, to ensure constant final (end-compression) conditions in the main chamber, initial pressure was varied. Hence the average Reynolds number increased as clearance was increased. Therefore our approach (which are based on the mid-pressure $Pe$ as a surrogate for the average) would predict an increasingly homogeneous final state as final clearance is increased in this scenario, consistent with the direct results of Mittal et al.\textsuperscript{7}

The role of the corner vortex in temperature inhomogeneity of an RCM has two main stages. The first aspect is the formation of the roll-up vortex from the boundary layer during the compression phase. Crevice volume ratio $a$ is closely related to this process, since the main function of the crevice is to suppress formation of the the roll-up vortex during compression by swallowing the boundary layer. The second stage is mixing of the cool boundary layer into hot core gas, which is due to the development and propagation of any residual vortex. Aspect ratio $b = D/(2S)$ in the final correlation characterises the space
available for cooler roll-up vortex to move from the corner towards the centreline and mix cool wall gas with hot core gas. The results of CFD simulations show that the aspect ratio has a larger effect than crevice volume ratio.

The apparent secondary importance of crevice volume ratio is due to the role of the crevice in suppressing the roll-up vortex, which is just one mechanism of overall temperature inhomogeneity. The thermal boundary layers also make a large contribution, which becomes dominant when the crevice is large. At long post-compression time, the influence of the crevice volume becomes negligible, as expressed in the correlation for $\bar{\varepsilon}_{\infty}$. The direct influence of crevice volume is small, but the correlation as presented does not account for the practical difficulties that researchers operators may encounter in adjusting an RCM. The crevice volume may be less constrained than other parameters such as piston velocity or diluent gas composition, and thus can yield a larger impact than a simple comparison of the exponents in the correlation would suggest.

Because of the large number of simulations and high computational costs for development of a correlation, some details have been simplified in this study. The sensitivity analysis does not consider non-linear effects or interactions between dimensionless parameters (although the full parametric study confirms the relative importance of the variables, as predicted by the sensitivity study, for the four variables retained). The methodology should be extended in future to study the interactions and non-linear effects of dimensionless parameters. Pre-compression temperature inhomogeneity (stratification) due to uneven wall heating or chamber filling, piston mis-timing, and three-dimensional effects (e.g. due to filling ports) could be investigated. The contributions of boundary layer formation and vortex-enhanced mixing to overall inhomogeneity could be differentiated in future work. Systematic optimization of crevice and entrance channel geometry could be undertaken with aid of automated simulations. Recent experimental\textsuperscript{18} and theoretical\textsuperscript{19} works suggest that turbulence may be significant and large eddy simulation should be considered in future studies supported by experimental measurements.
6 Conclusions

A simplified framework has been presented for prediction of temperature inhomogeneity in RCMs. The approach is applicable to any RCM configuration and any gas mixture properties. It is based on a definition of a reduced set of variables that govern inhomogeneity, by systematic elimination of many variables that are redundant or insignificant. A dimensionless measure of temperature inhomogeneity was defined and found to be primarily dependent on only three dimensionless parameters, the Peclet number $Pe$, aspect ratio $b$, and crevice volume ratio $a$, in order of decreasing importance. Temperature inhomogeneity has been computed by simulation over the full range of these parameters. Specific trends observed in the present work are in agreement with previous research, but the dimensionless framework is more comprehensive in mapping the RCM parameter space than any previous work, and permits simple and general application. The computational results are well modelled by a simple correlation

$$\bar{\varepsilon}_p(Pe, a, b, t^*) = \bar{\varepsilon}_\infty - (\bar{\varepsilon}_\infty - \bar{\varepsilon}_{0p})e^{-\beta t^*}$$

where

$$\beta = 3.08 Pe^{-0.32}a^{-0.08}b^{-0.40}$$

$$\bar{\varepsilon}_{0p} = 1.49 Pe^{-0.47}a^{-0.07}b^{-0.63}$$

$$\bar{\varepsilon}_\infty = 1.66 Pe^{-0.22}b^{-0.33}.$$  

These equations enable prediction of inhomogeneity in any RCM (within the broad range of parameters considered) up to time $t^* = 12$ post-compression, or 200 ms in our machine.

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