Development of a Three-dimensional Transient Wall Heat Transfer Model of a Rotating Detonation Combustor

Arnab Roy[1,*,‡], Clinton Bedick[2,*,†], Peter Strakey[3,*], Todd Sidwell[4,*], Don Ferguson[5,*]

Andrew Sisler[6, †,*], Andrew Nix[7,†]

**National Energy Technology Laboratory, Morgantown, WV 26507*

[‡]*AECOM, Morgantown, WV 26507*

[†]*West Virginia University, Morgantown, WV 26505*

Numerical simulation of transient heat transfer characteristics of a Rotating Detonation Combustor (RDC) is presented in this paper. A three-dimensional transient conduction model was developed to study the effect of large variation, periodic gas temperature exposed to the inner walls of the rotating detonation combustor outer body. The objective of the simulation is to predict heat flux transients and the interior wall surface temperatures from start up to 10s operation. The time varying, three-dimensional periodic convective boundary condition used for the heat transfer simulation is representative of the detonation wave propagation and other physical characteristics of RDC operating around 3000Hz and is derived from a separate computational fluid dynamics (CFD) simulation. The complex flow distribution downstream of the detonation/fill region results in a wall temperature and fluid dynamics that varies temporally and spatially in all directions. Simulation results were compared with experimental temperature data from literature on the outer body of an uncooled RDC. Combustor wall temperature variation in the axial direction indicates effect of non-uniformity on gas temperature distribution in the combustor for a non-premixed geometry. The simulation provides an estimate of transient heat load and hot spot locations that are critical to design efficient combustor cooling strategies.

Nomenclature

C	=	Specific Heat Capacity (kJ/kg-K)
CFD	=	Computational Fluid Dynamics
D_T	=	Thermal Diffusivity (m^2/s) = $k_{wall}/(\rho_{wall}C)$
htc	=	Heat transfer coefficient (W/m^2-K)
k_{wall}	=	Thermal conductivity of wall (W/m-K)
RDE	=	Rotating Detonation Engine
RDC	=	Rotating Detonation Combustor
t	=	Time (s)
T	=	Temperature (K)

[1] Research Engineer II, AECOM, AIAA Member, arnab.roy@netl.doe.gov
[2] Research Engineer, West Virginia University Research Corporation, clinton.bedick@netl.doe.gov
[3] Senior Research Engineer, AIAA Member, peter.strakey@netl.doe.gov
[4] Research Mechanical Engineer, AIAA Member, todd.sidwell@netl.doe.gov
[5] Senior Research Engineer, AIAA Member, donald.ferguson@netl.doe.gov
[6] Graduate Student, West Virginia University, AIAA Member, andrew.sisler@netl.doe.gov
[7] Assistant Professor, West Virginia University, AIAA Member, andrew.nix@mail.wvu.edu

x, y, z	=	Cartesian co-ordinates (m)
θ	=	Angular co-ordinate (rad)
ω	=	Angular wave speed (rad/s)
τ	=	Final time (s)
ρ	=	Density of outerbody wall (kg/m^3)

I. Introduction

TURBINE inlet temperature and pressure are key parameters in determining the thermal efficiency and work extraction capability of a gas turbine engine. Radical improvements in turbine component material and thermal management strategies have revolutionized gas turbine design over the last few decades. As a result, modern gas turbine engines operate at turbine inlet temperatures higher than alloy melting temperatures and achieve greater efficiency. However, opportunities for further improvement exist as even with state of the art combined power cycle gas turbine technology, power generation cycle thermal efficiency is still much lower compared to the ideal theoretical maximum – the Carnot Engine efficiency. Therefore, there is a need to identify sources of significant losses within the system and further investigate in detail the loss generation mechanism in order to mitigate. While combustion efficiency is typically high, the combustion process in a gas turbine Brayton Cycle contributes significantly to entropy generation and thus warrants greater attention for further improvement. Pressure gain combustion (PGC) is a promising technology that has the capability to provide a transformational increase in work availability (less entropy generation) and thermal efficiency compared to a conventional gas turbine combustor which relies on stationary deflagration combustion leading to pressure loss across the combustor. PGC utilizing a detonation pathway resulting in near constant volume combustion as described by the Zeldovich-von Neumann-Doring (ZND) cycle produces comparable gas temperatures while achieving an increase in pressure across the combustor. Pulse Detonation Engine (PDE) and Rotating Detonation Engine (RDE) are two primary variants of detonation based PGC technology. While PDE's have been widely studied[1], RDE's have gained renewed attention in recent years[2] due to simpler design that eliminates the need for a complicated valve mechanism and deflagration to detonation (DDT) devices, and potential advantage with regards to integrating with turbine stages due to nearly steady combustor exit conditions.

Combustor thermal management and heat transfer analysis is critical to safety and reliability of an RDE for long duration operation without exceeding material limitations. The RDE is essentially a cylindrical annulus where reactants are fed along the axial direction with a sustaining detonation wave, once initiated, rotating in the azimuthal direction at a relatively high operating frequency dictated by the combustor geometry and fuel/air inlet conditions producing a quasi-steady exit flow from the combustor. The high amplitude heat release within the traveling detonation zone may be detrimental to the combustor walls as well as downstream components. Therefore, accurate prediction of heat transfer parameters – surface temperature and heat flux distribution – is necessary to incorporate appropriate cooling methods.

Bykovskii et al.[3] reported the first known heat flux measurements in an operational RDE and concluded that although the average heat fluxes to the combustor walls are similar in case of detonation and a conventional gas turbine combustor using deflagration, the peak heat flux can be 2-3 times higher. They identified the critical region experiencing highest temperatures is within the detonation region between the leading shock front and detonation front. Frolov et al.[4] presented inner and outer wall temperature and heat flux transients using 3-D CFD simulations. These simulations showed that inner wall heat fluxes were greater than the outer wall and the difference increases with inlet pressure and temperature. Theuerkauf [5] performed heat flux measurements on both uncooled and water cooled RDEs using thin film gauges. While no concrete conclusions could be made from uncooled experiments due to the relatively short duration of the tests and life of the thin film gauges, the data obtained from water cooled RDE rig showed much higher peak heat fluxes and detonation wave speed greater than 3000m/s suggesting the possibility of multiple detonation waves propagating within the combustor. This would seem to exacerbate the need for a better understanding of the heat flux within an RDE device as the occurrence of multiple detonation waves could produce greater thermal stress. More recently, Randall et al.[6] presented experimental data on wall temperature distribution at different depths from the inner surface of the outer body. The temperature measurement was performed with standard (relatively slow responding) thermocouples and was complimented by a 3-D transient axisymmetric heat transfer model to predict wall temperature evolution. However, the time step used in this simulation was 0.1s suggesting that detonation timescales have not been well resolved.

The brief description of the background research summarized above clearly indicates the need for better characterization of the transient heat transfer processes experienced by the combustor walls in an RDE. Prediction of surface temperature and peak heat fluxes are critical to assess coolant requirements and future design considerations for RDE devices. The present study elaborates on the development of a 3-D heat transfer model using open source simulation software OpenFOAM© with time and space varying convective boundary condition derived from a more complex 3-D CFD simulation of Rotating Detonation Combustion (RDC). Coupling the wall heat transfer characteristics of the RDC flow-field consisting of detonation, oblique shock, combustion and other complicated phenomena in a computationally efficient and inexpensive manner was the major motivation behind development of the OpenFOAM model. Details of the model development procedure are outlined in the next section followed by detailed discussion on the results obtained thus far.

II. Heat Transfer Model Description

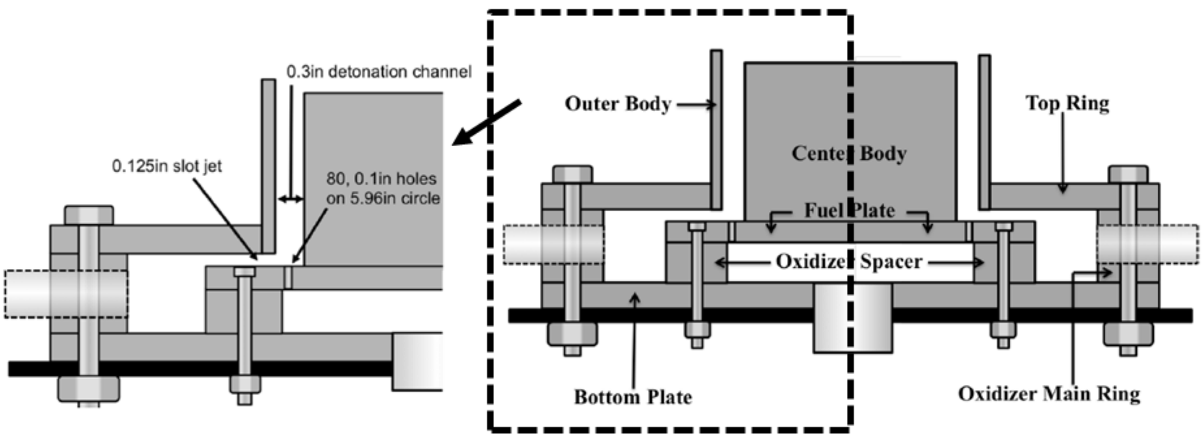


Figure 1: Modular RDE developed by Shank et al.[7]

Figure 1 shows the RDE geometry[7] that has been chosen as the base case design for heat transfer model development. The first step is to carry out 3-D unsteady RANS simulation of the RDC flowfield using ANSYS-Fluent© up to stable detonation operation of 2-3 cycles. Details of the CFD mesh and simulation are provided in Roy et al.[8] and therefore are not repeated here.

The heat transfer model geometry consists of the outer body shell including the inner surface and outer wall of the RDE as shown in Fig. 1. The outerbody material was taken to be 316 stainless steel with a height of 5.125 inches. The outer and inner radii were 3.03 inches and 3.322 inches, respectively, resulting in an outerbody thickness of 0.292 inches. In general, describing the transient thermal response within a solid, isotropic material is relatively straightforward, however determination of appropriate and representative boundary conditions can be challenging. The temperature distribution was modeled within the outerbody wall of the RDE in three dimensions using the OpenFOAM LaplacianFOAM solver. LaplacianFOAM solves the Laplace equation for isotropic, unsteady heat conduction, as shown in Eq. [1].

$$\frac{dT}{dt} - \nabla^2(D_T \cdot T) = 0 \qquad [1]$$

Where, D_T is the thermal diffusivity of the RDE outerbody wall material. The upstream and downstream surfaces of the RDE along with the outer surface boundary conditions were considered to be adiabatic. While this simplifies the analysis, natural convective boundaries would have been more accurate and will be implemented in future studies.

As mentioned earlier, time varying gas temperature data obtained from a full CFD simulation using ANSYS-Fluent RDE were utilized for the inner surface boundary condition. As the combustion and wall heating processes are being modeled separately, this approach will only allow 1-way coupling of the fluid-solid thermal interactions. However because the gas temperatures are in general much higher than the wall temperatures and due to the highly transient nature of the heating, it is expected that the wall heating will minimally affect the fluid dynamics and chemistry for the simulation times being considered. Due to the computation expense of modeling detailed chemistry and turbulence with time scales on the order of microseconds, the simulation models consists of a few milliseconds of physical time. However, given the high frequency of the travelling detonation wave this provides an adequate representation of the highly non-uniform temperature and pressure distributions within the RDE combustion annulus which varies in time and space (axial and circumferential). Utilizing the periodic nature of the gas temperature profile, a line of sample points were positioned in the axial direction and temperature data were extracted over a period representative of a complete revolution of the detonation wave. Assuming stable, periodic behavior of the working fluid, the gas temperature data were then extended in a periodic manner so that OpenFOAM simulation times of several seconds could be considered. It was important to maintain time steps close to CFD simulation in order to fully resolve gas temperature transients.

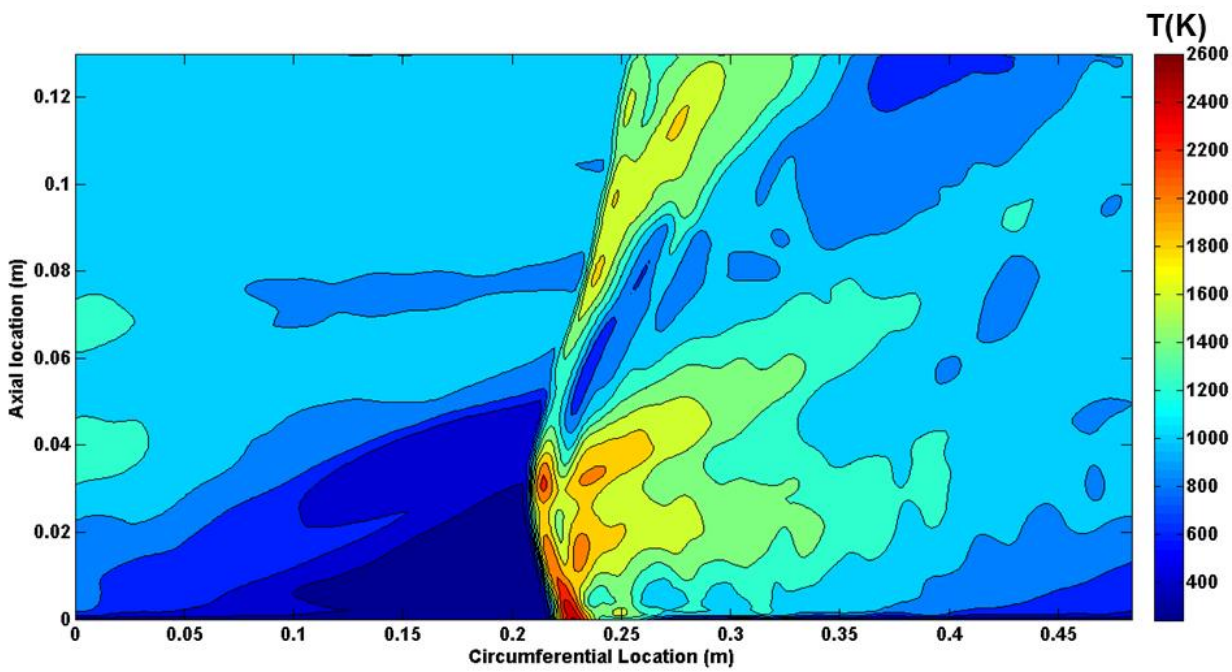


Figure 2: Unwrapped RDE 2D gas temperature profile

In order to fully map the data from CFD simulation output in OpenFOAM, interpolation must occur at each cell on the inner boundary based on each boundary cell's axial and circumferential position, as well as the current simulation time. The RDE angular position for each boundary cell, *i*, relative to the geometric orientation shown in Figs. 1 and 2, is determined by Eq. [2] as:

$$\theta_i = tan^{-1}(x_i/z_i) \qquad [2]$$

In addition, the computed angles are wrapped from 0 to 2π. The cell circumferential positions are converted to time-dependent values so that as the simulation advances, the data profile is shifted circumferentially around the RDE outerbody inner surface. In order to implement this, the average angular wave speed must be known, determined by Eq. [3], where Δt is the time taken to complete 1 revolution by the detonation wavefront.

$$\omega = \frac{2\pi}{\Delta t} \qquad [3]$$

The angular wave speed was determined from RDC operating frequency. The time variable used for interpolation of the gas temperature data at each boundary cell, *i*, is determined by Eq. [4], where *t* is the current simulation time.

$$\tau_i = t + \frac{\theta_i}{\omega} \qquad [4]$$

$$\begin{aligned} \tau^*{}_i &= \tau_i & & if\ \tau \leq t_{max} \\ \tau^*{}_i &= fmod(\tau_i, t_{max}) & & otherwise \end{aligned} \qquad [5]$$

As the simulation time increases, the time lookup variable calculated by Eq. [4] will eventually become larger than what is represented in the imported gas temperature data. In order to allow very long simulation times without the need for large data files, it was desired to repeat the data shown in Fig. 2 in a periodic manner throughout the simulation. This was accomplished for each boundary cell, *i*, using the C++ modulus operator (*fmod*) as shown in Eq. [5], where t_{max} is the maximum time represented in the imported gas temperature data and assuming the data begins at time t=0. Implementation of the time-dependent convective boundary condition was accomplished using the *codedMixed* boundary condition type within OpenFOAM[9]. The general *coded* boundary condition allows the user to develop a custom, arbitrary Dirichlet boundary condition by writing C++ code directly into the OpenFOAM boundary file for a given variable. The *codedMixed* boundary condition adds the capability of providing a Neumann or mixed boundary condition. For the RDE simulations here, a strictly Neumann boundary condition was applied, based on the Fluent gas temperature data shown in Fig. 2. At runtime, the *coded* or *codedMixed* boundary condition is compiled and called by the solver. This approach allows complete freedom with regards to the implementation of mathematical expressions, access to solver variables, and use of other OpenFOAM libraries.

In order to determine appropriate instantaneous gas temperature values, a two-dimensional interpolation scheme was implemented using the available OpenFOAM 2D interpolation table library, *interpolation2DTable*. After appropriately formatting the desired data in a text file and providing the filename to the interpolation2DTable variable constructor, gas temperature values at each boundary cell, *i*, can be easily interpolated using any variable pairs contained within the tabulated data. Additional details regarding *interpolation2DTable* usage can be found in the OpenFOAM source guide[9]. Finally, the *gradientExpression* function used at the inner wall in OpenFOAM is shown in Eq. [6].

$$\left.\frac{dT}{dn}\right)_i = \frac{htc * (T_{gas} - T_{wall})}{k_{wall}} \qquad [6]$$

where *n* is a local coordinate normal to the wall, *htc* is convective heat transfer coefficient (assumed constant for simplification) and T_{gas} is fluid temperature adjacent to cell *i*.

Finally the unsteady heat transfer simulation was carried out upon application of the above boundary conditions as discussed above for the prediction of RDE outerbody wall temperatures at significantly longer simulation times (4s-10s) with reduced computational effort. In addition, the existing OpenFOAM parallel execution capabilities allow running simulations on the NETL HPCEE cluster, further reducing run times. For example with 200k elements, on 32 processors with time steps between 5 - 10μs, ten second simulation run time can be completed within two days. The solution was tested for grid independence and time-step sensitivity was also checked.

Table 1: Model parameters

Material Property Values		Physical Parameter			Row#	Co-ordinates (mm)
k **(W/m-K)**	D_T**(m²/s)**	T_i **(K)**	***htc*** **(W/m²-K)**	**Δ*t*(s)**	**1**	**(76.795, 31.25, 0)**
16.2	**4.034 x 10⁻⁶**	**300**	**500**	**5μs for t = 4s**	**2**	**(76.795, 57.15, 0)**
			1000	**10μs for t = 4s**	**3**	**(76.795, 82.55, 0)**
			2000	**-**	**4**	**(76.795, 107.95, 0)**

III. Results

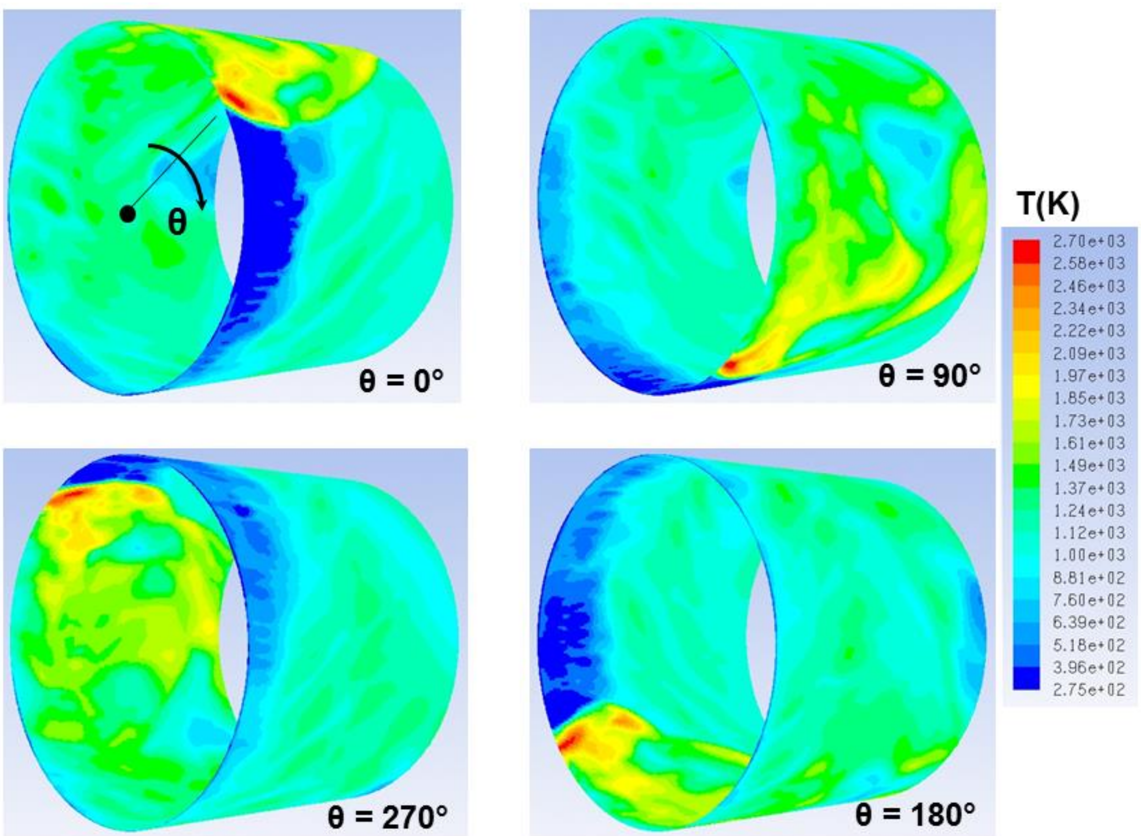
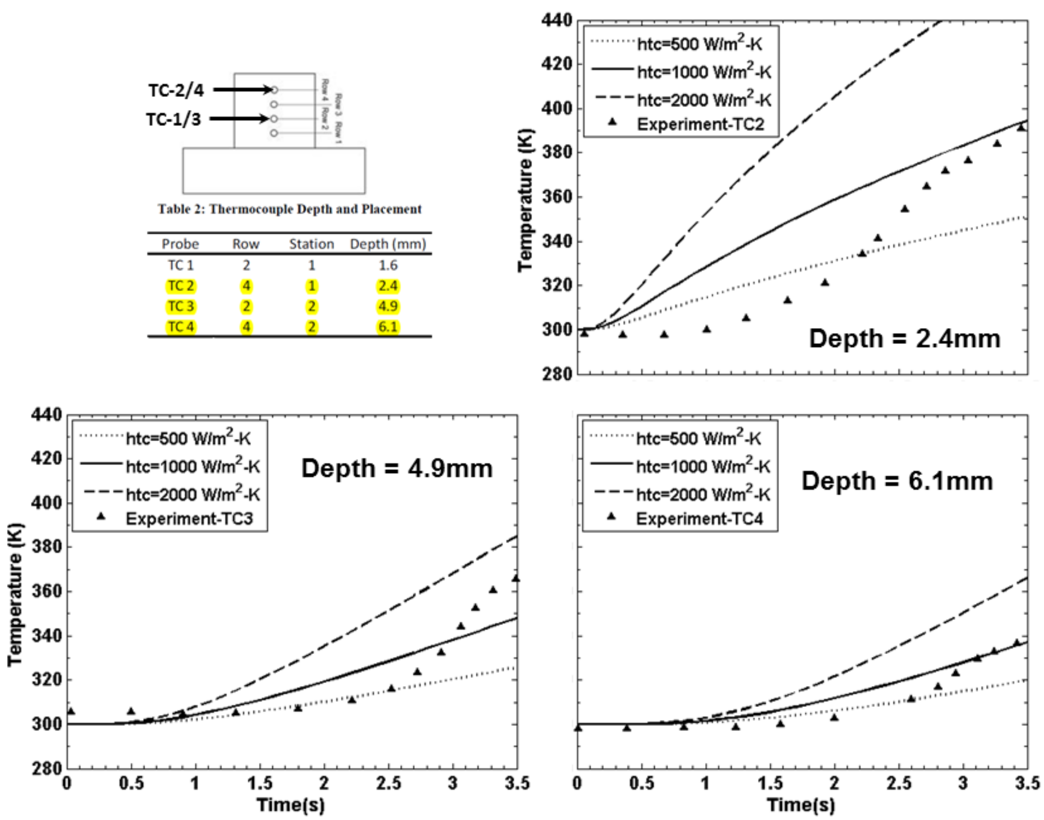


Figure 3: CFD fluid temperature contour plot adjacent to outerbody inner surface (1 cycle)

Figure 3 shows a color plot of gas temperature in the annulus region adjacent to the outerbody wall for the RDC operating with 0.5 kg/s air flow rate (Eq. ratio ~ 0.97) and atmospheric exhaust pressure condition. For the heat transfer simulation, the temperature distribution at the inner wall of the outerbody was used as boundary condition.

These figures demonstrate some of the key flow features such as detonation wave, expansion region, and post-detonation oblique shock that occur within the RDE. The dynamic nature of these flow features complicates assumptions associated with convective heat transfer. Randall et al.[6] presented a basis for correlating the heat transfer coefficient to Nusselt number that would account for the highly dynamic flow field of the RDE. However, that study ultimately deferred to experimental studies with measured heat fluxes to estimate a possible range of heat transfer coefficient values (*htc* [W/m^2-K]: 500 -2000). These values were also utilized in the current study however it should be noted that given the variability of empirical data and the uniqueness of the flow field within an RDE, the level of uncertainty regarding the heat transfer coefficient could be significant.

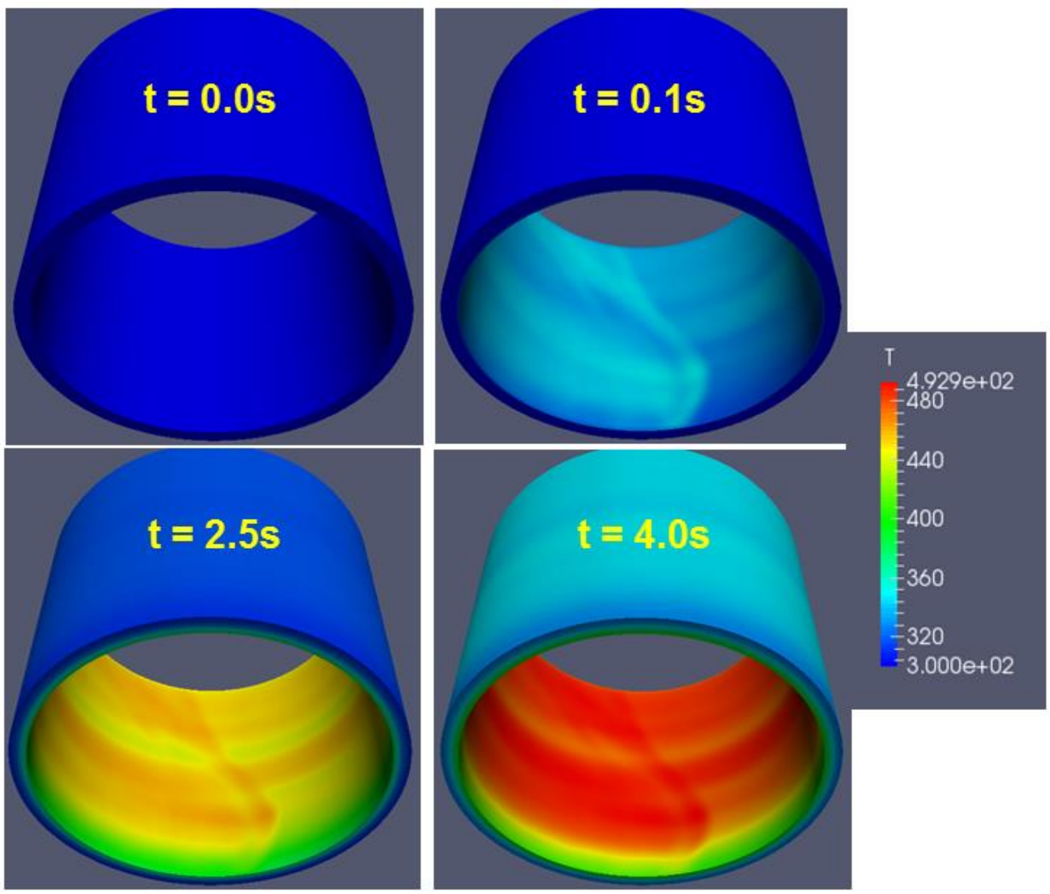
Comparison between experimental data obtained by Randall et al.[6] and the present model is shown in Fig. 4 for a range of heat transfer coefficients as previously described. In their study Randall et al.[6] voiced concern over the accuracy of data from TC1 and thus it was not be included in this comparison. Although trends vary between the experimental and numerical studies,Fig. 4 shows reasonable agreement in predicting the final wall temperature (*htc* = 1000 W/m^2-K) at all locations (TC2, TC3 and TC4). This study is also a further development from earlier publication[8] where 1-D analytical and 2-D numerical model was developed and compared against the same experimental dataset. The comparison shown in Fig. 4 and as presented in Roy et al.[8] with the 2-D model exhibit similar trends, however implementing the periodic gas temperature transients experienced by the outer body wall is a more logical approximation compared to a periodic heat flux boundary condition. Again it should be reiterated that the wall heat transfer coefficient used in convective boundary condition is expected to vary significantly within the entire combustor domain and be strongly influenced by wall temperature rise over time; however, it is kept constant for simplicity in the present study.



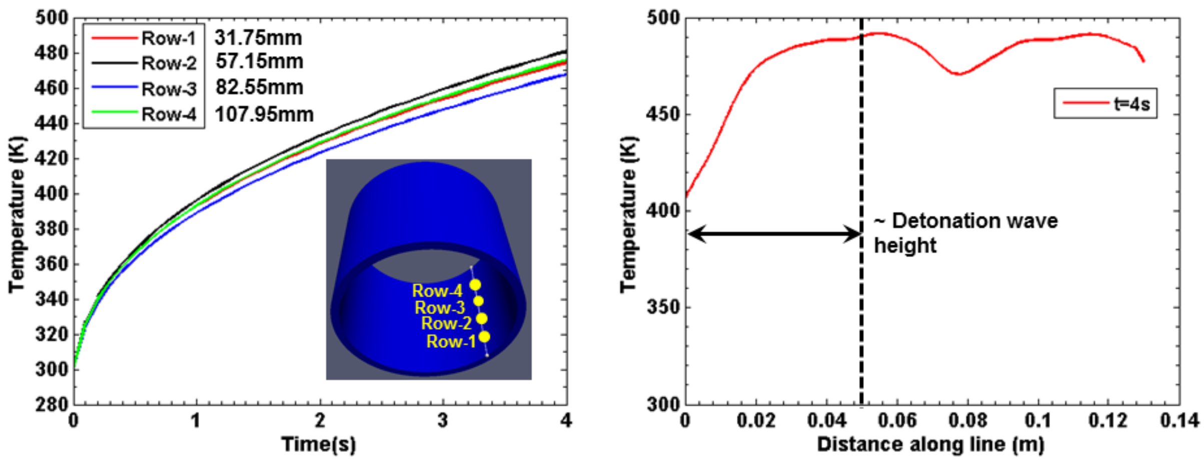
Probe	Row	Station	Depth (mm)
TC 1	2	1	1.6
TC 2	4	1	2.4
TC 3	2	2	4.9
TC 4	4	2	6.1

Figure 4: Comparison of 3D numerical model with experimental data[6] at different depths of combustor wall from inner wall (a) TC2 = 2.4mm, (b) TC3 = 4.9mm, (c) TC4 = 6.1mm

Figures 5(a) and (b) represent time history of wall temperature variation in the RDC outerbody (3D color plot) and at four locations along a line on the inner surface in the axial direction. The co-ordinates of these locations (Row-1 to 4) are provided in Table 1. The color plots in Fig. 5(a) clearly show the strong influence of gas temperature on spatial distribution of wall temperature as the rotating detonation wave, oblique shock wave, deflagration regions and other dominant flow features are evident. As the RDC operation time increases, heat fluxes penetrate further into the combustor walls resulting into a more diffused temperature distribution. Figure 5(b) indicates that increases in wall temperature along the axial direction is highly non-uniform and it can be identified that the primary hot spot region in the combustor wall occurs some distance downstream of the detonation zone (primarily near the triple point region). It is also revealed from Fig. 5(c) that the effect of regenerative cooling in the dump-plane region due to the fill zone (fresh incoming fuel-air mixture) ahead of the detonation wave is restricted up to 40% detonation height (approximate detonation height from CFD simulation is 50mm). This is significantly lower compared to all cases studied earlier and is evident as Row-1 (within detonation zone) and Row-4 (near exhaust zone) temperatures are almost similar.



(a)

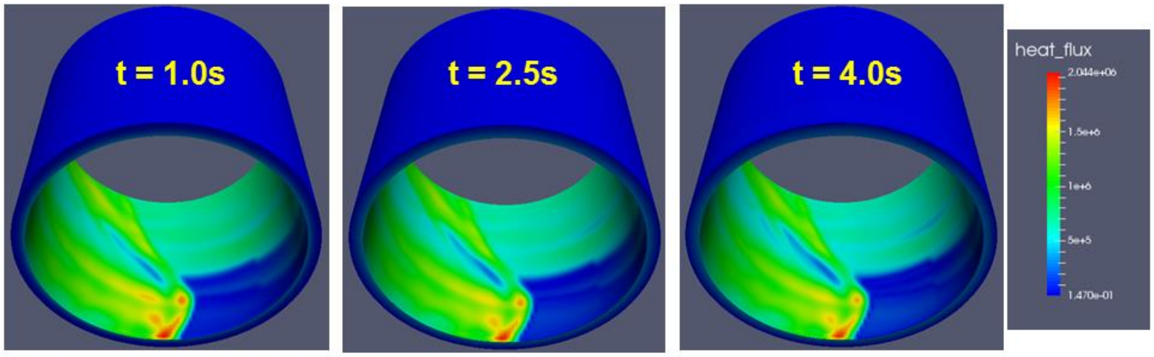


(b) (c)

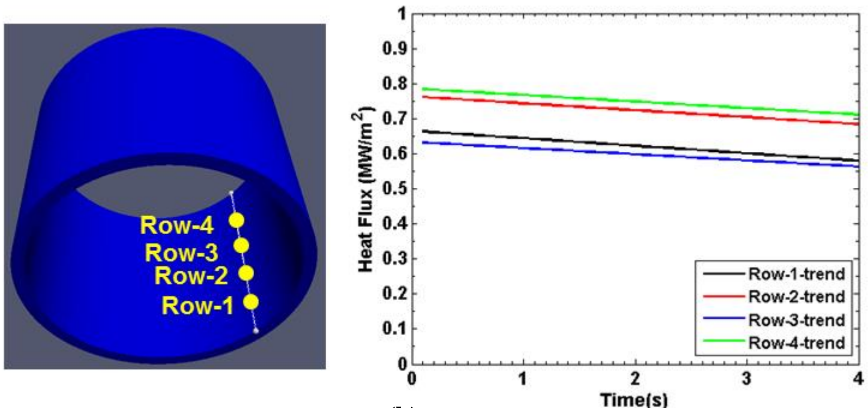
Figure 5: (a) 3D contour plot of wall temperature plots at different time instants, (b) time history of wall temperature at four locations Row-1 to 4, (c) temperature variation along axial direction at t=4s

Commonly, it has been observed in premixed simulations that the triangle shaped fill zone consists of fresh fuel-air mixture at very low temperatures (temperature drop ~ 50-70°K), caused by sudden rapid expansion of air at supersonic conditions. In case of a non-premixed injection scheme, due to poor mixing there is no distinct fill zone boundary and losses are incurred due to several local combustion regions which increases the overall temperature of the fill zone mixture, therefore resulting in reduced cooling effect. However, whether this effect is primarily due to the difference in fuel-air injection type (premixed vs non-premixed) or specific to the RDC design can only be confirmed when a premixed simulation is performed with identical flow conditions and a comparison is made – which will be reported in future work.

Transient heat flux to the RDC outerbody wall is calculated using the solution variables and mean temporal variation at specified locations along axial direction are illustrated in Figs. 6(a) and (b) respectively. It can be seen from heat flux color plots that the highest load (~2 MW/m^2) occurs near the region behind the detonation wave front and decreases with time as expected due to increase in surface temperature. Average heat flux variations at Row-1 to 4 locations along the axial direction shown in Fig. 6(b) are estimated to be 0.5MW/m^2 - 0.8MW/m^2. It is also observed that the difference between detonation and exhaust region unsteady heat flux variation is minimal.

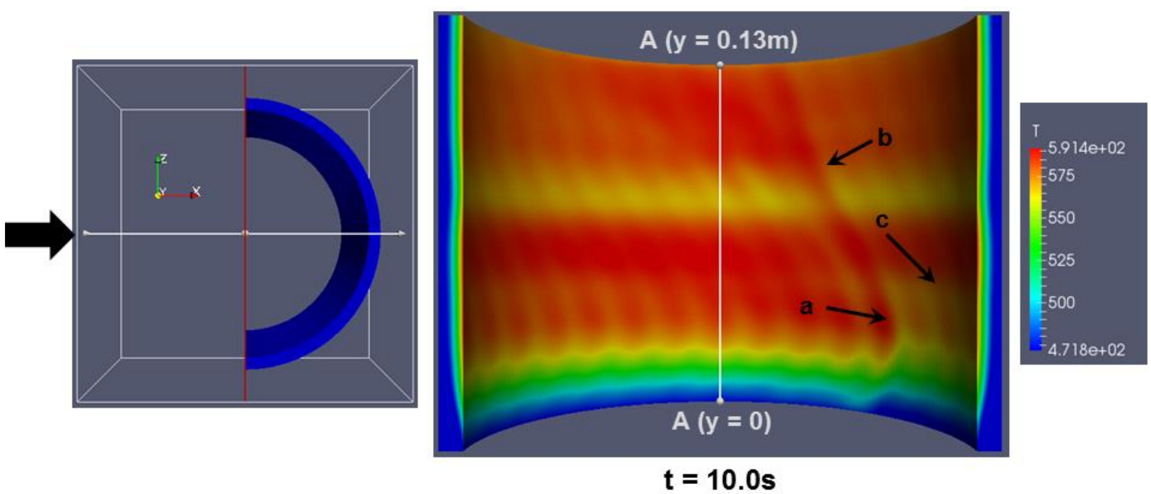


(a)

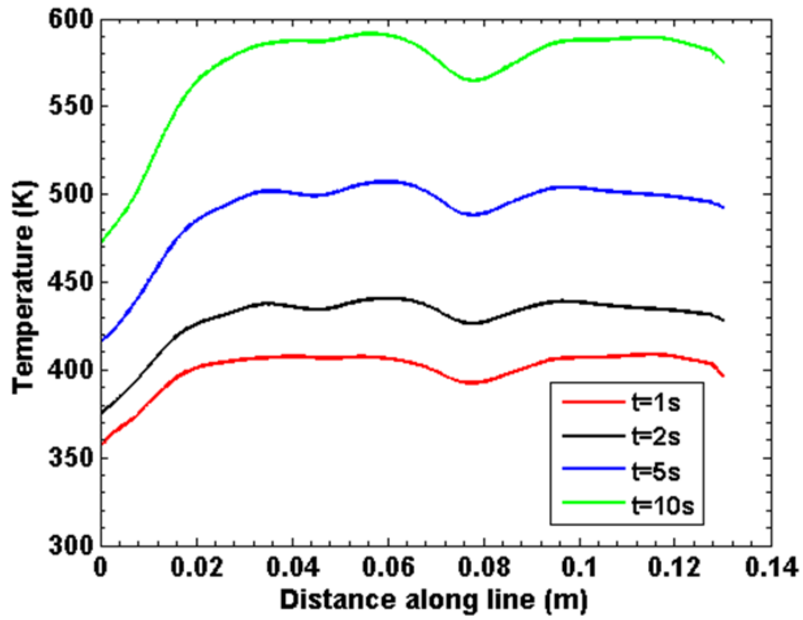


(b)

Figure 6: (a) Calculated Heat flux contour plot during RDC operation, (b) mean temporal heat flux variation at Row-1 to 4 locations



(a)



(b)

Figure 7: (a) Mid-section 3-D temperature plot at 10s of RDC operation showing instantaneous location (a = detonation wave, b = oblique shock wave, c = deflagration boundary), (b) wall temperature evolution in the axial direction along line A-A

Figure 7 shows 3-D temperature distribution of the RDC outerbody after 10s run duration clipped at mid-section. This simulation was run with 10µs time step to lower simulation run time, however it should be noted that with a 10µs time step there may be a possibility of skipping the peak gas temperature value within a cycle, as at some locations the rise time to peak gas temperatures is ~7-10µs. The CFD simulation was performed with 1µs time step for two steady RDC operating cycles. The maximum surface temperature predicted is ~ 593K after 10s. The axial temperature distribution shown in Fig. 7(b) along the line through Row-1 to 4 follows similar pattern and is a further extrapolation of data presented in Fig. 5(c).

IV. Conclusions and Future Work

Three-dimensional heat transfer model of an RDC outerbody wall has been developed using open source simulation software OpenFOAM© with a transient periodic convective boundary condition. Gas temperature at the inner surface of the outerbody has been mapped directly from a 3-D CFD simulation carried out using ANSYS-Fluent© under steady operation for 2 cycles and a periodic condition is implemented in the heat transfer model to match the desired RDC frequency and time duration. The major objective of the present study is to isolate the wall heat transfer characteristics from a more complex and computationally expensive conjugate thermal simulation. Preliminary results have been compared with available experimental data and important findings were discussed in detail. The regenerative cooling near the inlet due to fill zone was shown not to be sufficient to cool combustor walls up to the entire detonation height, as wall temperatures after 40% detonation height were similar to RDC exhaust region for 4s-10s operation. Predictions indicate that for this specific uncooled RDC design, peak and average heat fluxes were ~ 2-2.5 MW/m^2 and 0.5-0.8 MW/m^2 respectively with a maximum wall temperature ~600K after 10s operation. Further development of the OpenFOAM model is in progress, where time dependent material properties and spatial variation of heat transfer coefficient will be implemented. The present model developed will also aid as a predictive tool for hot spot identification and heat flux estimation for in house NETL-RDC experiments as well as support thermal management strategies of other RDC designs available in literature.

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