NUMERICAL COMPUTATION OF TURBULENT COMBUSTION AND THERMAL RADIATION IN GAS TURBINE COMBUSTION CHAMBERS

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ABSTRACT

The numerical simulation of the radiative heat-transfer in reacting flows in aircraft gas turbine combustion chambers is presented. The radiative heat-transfer process is modelled by extending the Discrete-Transfer Method\cite{1} to arbitrary geometries. The modified scheme uses a ray tracing technique in general curvilinear coordinates. The model equations for the reacting flows are the Favre averaged Navier-Stokes equations together with the two-equation $k-e$ turbulence model. The mean reaction rate is handled through the use of the Eddy Dissipation Concept model\cite{2}. The flow calculations are performed using a fully second order finite difference scheme. The results show that heat radiation plays an important role in temperature distributions. It was found that the relative importance of the radiative heat-transfer is different for different flame situations. In particular, it is more important in flames with low flow speed. Different shapes of the presumed probability density function have also been examined.

1 INTRODUCTION

Radiative heat-transfer is believed to be one of the important heat-transfer mechanisms in combustion chambers, such as gas turbines\cite{3,4,5}. For engineering applications, an important question is the contribution of heat-radiation to other energy transfer/production processes: advection, conduction, and heat-production due to chemical reaction. It is also evident that due to the non-linear dependence of the chemistry on the local temperature, the total effect of energy-transfer can not be simply super-posed. Radiation plays an important role in heat transfer: without radiative-heat transfer one would see much higher local temperatures, which by itself would result in significant increase in the formation of NO2. The effects of radiative heat-transfer are important from engineering point of view. It is also clear that the geometry of the combustion chamber plays an essential role for radiative-heat transfer. Other factors that determine the temperature in a combustion chamber are the location and extent of the flame soot formation, and the mode of combustion (e.g. staging). It is, however, not uncommon that the effects of heat radiation are neglected, by which one can simplify the analysis (e.g. the analysis of the "flamelet" outer structure\cite{6,7}).

Calculation of radiation in an absorbing-emitting-scattering medium is difficult, since the governing relation is an integrodifferential non-linear equation. Some assumptions are usually adopted for engineering applications such as "grey gas", non-scattering, or isotropic scattering assumptions\cite{4,5}. Several methods have been proposed for solving the radiation intensity field: Monte-Carlo Method\cite{8}, Zonal Method\cite{9}, Finite Fluxes Methods\cite{10}, Finite Volume Method\cite{11} and Discrete Transfer Method (DTM)\cite{11}. Extensive reviews on various methods are given in references\cite{3,4}. Our effort here is concentrated on applying an extended DTM to reacting flows in complex geometries and studying the relative importance of radiation in calculation of turbulent reacting flows in gas turbine combustors.

The DTM proposed by Lockwood and Shah\cite{11} consists of the following steps: The boundary of the domain is discretized into small area segments (cells). The radiative flux impinging on a boundary cell is discretized into a finite number of rays with associated solid angles. The ray travelling in the medium starts at some other boundary cell. The ray path is identified by some ray-tracing technique. The equation of radiative flux intensity is discretized and integrated along the path of the ray (assumed to be straight). When the intensity field is solved, the source term in the en-
ergy equation due to radiation can be computed. The key issue for DTM is the calculation of ray paths in a complex geometry with (fully or partially) reflecting boundaries. In section (3.2), we propose a "ray-tracing" technique that can be applied to general 3-D problems.

The radiation calculation has been integrated into a three dimensional reacting flow solver\cite{[12]}. The model equations used in the solver are the Favre averaged Navier-Stokes equations together with the two-equation $k-\epsilon$ model. The interaction between chemistry and the turbulent fluctuations was modeled using the Eddy Dissipation Concept model\cite{[2]}. These governing equations are solved using a second order finite difference scheme\cite{[14]}. The interaction between turbulence and radiation has to be accounted for. This has been less addressed in the current literature. Here, we consider the usage of the presumed Probability Density Function (PDF) to account for the effect of the fluctuating temperature field on the radiative intensity. Some different types of the PDF shape have been investigated (in section 4.2).

Using the above mentioned models and numerical methods, we performed calculations in cylindrical shaped combustion chambers (a gas turbine combustor) with non-premixed fuel (methane) and air supply. The relative importance of the radiative heat-transfer in the calculation of the flame temperature profiles in different flame situations has been examined, and it was found that the temperature field could be overpredicted by more than 10% when neglecting heat radiation.

2 Governing Equations for Turbulent Flames

The governing equations for turbulent flames are the Navier-Stokes equations together with the continuity equation, energy conservation equation, equation of state, as well as other supplementary equations. In the following, the equations for heat transfer are given, while the detailed description of the other governing equations are given in references\cite{[12]--[14],[15]}.

2.1 Models for Combustion in Turbulence

The Favre averaging process is applied to the Navier-Stokes equations and to the other transport equations that govern turbulent flows. The resulting unknown terms (e.g., the Reynolds stresses and the turbulent scalar fluxes) are modeled by the $k-\epsilon$ equations based on the eddy viscosity. The fuels employed here are Propane and Methane. A two steps reaction scheme\cite{[16]} is employed:

\[
C_nH_{2n+2} + \frac{2n+1}{2} (O_2 + 3.76N_2) \rightarrow nCO + (n+1)H_2O + (3.76n + 1.88)N_2
\]

\[
CO + 0.5(O_2 + 3.76N_2) \rightarrow CO_2 + 1.88N_2
\]

The reaction can be assumed to be "fast", so that the overall reaction rate is turbulence-controlled. We use the "Eddy-Dissipation Concept" of Magnussen\cite{[2]} to account for the turbulence-chemistry interaction, i.e., model the dependence of the mean reaction rate on turbulence.

2.2 Basic Equations for Heat Transfer

For studying the reacting flows at low Mach numbers with Lewis number equal to one, the energy conservation equation for steady flows can be written as

\[
\frac{\partial p u_j h}{\partial x_j} = \frac{\partial}{\partial x_j} (\mu \frac{\partial h}{\partial x_j}) - \nabla \cdot \mathbf{q}_R
\]

where the enthalpy is defined by

\[
h = Y_i h_i, \quad h_i = \int_{T_0}^{T} C_{P_i} dT + H_i^0.
\]

$H_i^0$ is the heat of formation of species $i$ at reference temperature $T_0 (\sim 25^\circ C)$. $Y_i, C_{P_i}$ are the mass fraction and the specific heat capacity of species $i$, respectively. $\rho, T$ are the gas density and temperature. $u_j$ is the velocity component in $x_j$ direction ($j = 1, 2, 3$). $\mu$ is the molecular viscosity. $P_r$ is the Prandtl number. $\mathbf{q}_R$ is the radiative heat-flux. The three terms, from left to right in Eq. (2) represent advection, conduction and radiative heat-transfer, respectively.

The term due to radiative heat-transfer is calculated by

\[
\nabla \cdot \mathbf{q}_R = \nabla \cdot \left( \int_0^\infty \int_0^{4\pi} \int \mathbf{i}'_s d\Omega d\lambda \right)
\]

\[
= \int_0^\infty \int_0^{4\pi} \frac{d\mathbf{i}'_s}{ds} d\Omega d\lambda
\]

where $s$ and $s$ are the coordinates and unit vector along the path of a ray, respectively. $\mathbf{i}'_s$ is the intensity of radiation at the wave length $\lambda$. The equation for the radiative transfer for an absorbing, emitting and scattering medium is\cite{[4]}:

\[
\frac{d\mathbf{i}'_s}{ds} = -a_s \mathbf{i}'_s + a_s \mathbf{i}'_{s \lambda} - \sigma_s \mathbf{i}'_{s} + \frac{\sigma_s}{4\pi} \int_0^{4\pi} \mathbf{i}'_{s} \Phi(\Omega, \Omega_s, \lambda) d\Omega_s
\]
where $a_\lambda$, $\sigma_\lambda$ are the absorption and scattering coefficients at the wave length $\lambda$, respectively. $\Phi(\Omega, \Omega_\lambda, \lambda)$ is the phase function for scattering, and $i_{\lambda\Omega}$ is the black body radiation intensity.

We adopt the assumptions of diffuse grey gas and non-scattering medium. These assumptions are adequate in the sense of averaging in the $\lambda$ space. Eqs. (4), (5) can be then simplified to

$$ \nabla \cdot \mathbf{q}_r = \int_0^{4\pi} \frac{dl}{ds} d\Omega $$

$$ \frac{dl}{ds} = \sigma_a (-I + \sigma T^4) $$

where $I$ and $\sigma_a$ are the radiation intensity and absorption coefficient of the diffuse grey gas. $\sigma = 56.7 \times 10^{-12}$ [kWm$^{-2}$K$^{-4}$] is the Stefan-Boltzmann constant.

The absorption coefficient is a function of composition, temperature, pressure, mean beam length[5], etc. The method of computing the absorption coefficient is given by Modak[17]. In reacting flow calculations, one has to solve the coupled system (2), (6), (7) as well as conservation equations for mass, species, momentum in addition to the equations used for modeling turbulence.

The boundary conditions for $I$ in (7) are specified by computing the total influx energy into a given control surface area, and the amount of radiated energy (due to the surface temperature, and taking into account the emissivity of the surface). Thus, once the outgoing radiative energy is given, one may compute the radiative intensity $I$, and (7) can be integrated. At inflow/outflow boundaries, we assume no reflection.

2.3 HEAT TRANSFER IN TURBULENT FLAMES

Flows with combustion are practically always turbulent. Turbulence plays an essential role in combustion and heat transfer. In many engineering applications, one is mostly interested in the mean quantities of the turbulent field. By using the Favre average, the energy equation (2) can be written, in terms of the means and correlations of the fluctuations, as:

$$ \frac{\partial \overline{\rho u_i h}}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \frac{\mu}{P_r} \frac{\partial h}{\partial x_j} - \overline{\rho \omega_i \omega_j} \right) - \nabla \cdot \mathbf{q}_r $$

The overbars denote the ensemble (or time) averages and the tildes denote the Favre averages. The superscripts 'n' denote the fluctuations from the Favre averaged value. Equation (8) contains unknown terms, i.e., the turbulent heat fluxes $-\rho \overline{\omega_i \omega_j}$ and the mean radiative heat source $\nabla \cdot \mathbf{q}_r$. These terms are not known and can not be computed directly from basic principles (this is the so-called 'closure problem'). Therefore, one has to model these terms if equation (8) is to be solved. Various modeling approaches may be adopted, depending on the underlying assumptions that have been made. Modeling of the turbulent heat fluxes can be done using the transport equation of the turbulent heat fluxes (the second order closure[18]), where higher order (third order) correlations have to be modeled. The mostly used approach is to model the turbulent heat fluxes based on the eddy viscosity and gradient diffusion hypothesis, i.e.,

$$ \mu \frac{\partial h}{P_r \partial x_j} - \rho u_i u_j h'' = \frac{\mu + \mu_t}{P_r} \frac{\partial h}{\partial x_i} $$

where $\mu_t$ is the eddy viscosity, which can be computed from the turbulent kinetic energy ($k$) and the dissipation rate of the turbulent kinetic energy ($\epsilon$) ($k$ and $\epsilon$ can be computed using the two equation $k-\epsilon$ model, the detail is given in references[12]-[13]).

Here we are mostly interested in the calculation of the mean radiative heat transfer source term $\nabla \cdot \mathbf{q}_r$. Eqs. (6)-(7) show that in order to compute the mean radiative heat source, the mean radiative intensity $I$ has to be evaluated. Applying the ensemble average to Eq.(7), we have

$$ \frac{dl}{ds} = -\overline{\sigma_a I} + \frac{\overline{\sigma_a T^4}}{\pi} $$

Two unknown correlations $\overline{\sigma_a I}$ and $\overline{\sigma_a T^4}$ have to be provided or modeled. The first one is the correlation of the fluctuating properties of the medium (i.e., the absorptivity) and the radiative intensity. This term is difficult to model due to the limitations in measured data. Generally, the two correlations can be computed by the joint probability density function (PDF) $\rho(T, p, Y_i, ...)$ via the integration

$$ (\overline{\sigma_a I}, \overline{\sigma_a T^4}) = \int ... \int (\sigma_a I, \sigma_a T^4) \times $n \rho(T, p, Y_i, ...)dTdpdY_i...$$

The typical value of $\sigma_a$ is between 0.2 and 0.3 in most flame fields. To first approximation, one may assume that $\sigma_a$ only depends on the properties of the medium, and that it is independent of the turbulent fluctuations. Hence,

$$ \overline{\sigma_a I} = \overline{\sigma_a T^4} $$

$$ \overline{\sigma_a T^4} = \overline{\sigma_a} \int_0^1 (T_{min} + \tau(T_{max} - T_{min}))^4 \rho(\tau) d\tau $$

where $\tau = (T - T_{min})/(T_{max} - T_{min})$ is the normalized temperature. The subscripts max and min denote...
the maximum and minimum values, respectively. This simplification enables us to study independently the influence of fluctuating temperature field on the radiative intensity and on the radiation source term in the energy equation.

The following shapes of the presumed PDF, $\varphi(\tau)$, are considered: the $\delta$ function, the triangular distribution (in these two cases only the mean of temperature is recovered exactly), the $\beta$ function and the clipped Gaussian distribution[19]. In the latter two cases, the mean and the variance of the temperature field determine the PDF. Higher moments are then "extrapolated". In this sense, the presumed PDF involves the information of higher order correlations will yield better accuracy. However, in practice, correlations more than second order are very hard to model. The behaviour of different shapes of PDF will be discussed in section (4.2).

The mean of the temperature can be obtained from the energy equation and thermodynamic relations. The variance of the temperature field may be estimated by

$$\bar{T}^2 = \frac{\xi^2 \bar{T}^2}{(T_{max} - T_{min})^2}$$

where $\xi = \sqrt{\bar{T}^2 / \bar{T}}$ is the relative intensity of the temperature fluctuations. $\xi$ may be computed through solving a transport equation; here we assume that $\xi$ is a global constant parameter for simplicity. We are mostly interested in the influence of different PDF shape on the radiation heat transfer.

Instead of a presumed PDF, one may solve a transport equation for the PDF. The transport equation for the PDF has been derived, as discussed by Pope[20]. This approach implies that some unknown terms (e.g. conditional expectations) must be modeled by employing certain physical assumptions. In addition, the need for solving an additional set of transport equations, which is usually time-consuming and requiring large computer capacity, makes the approach less attractive for applications that are not very sensitive.

3 Numerical Methods

The governing equations for reacting flows are solved numerically, using second order finite differences (second order upwind scheme for the advective terms; second order central differences for the other terms). A more detailed description of the scheme is given elsewhere[12]–[14]. In the following we shall describe the discrete transfer method that we have used for solving the radiative transfer equation (7).

3.1 The Discrete Transfer Method

The basic idea behind the discrete transfer method is as follows: Assume that the radiating rays arriving at boundary surface element $i (i = 1,...M)$ are represented by a finite number (i.e., $N$) of rays. The $I_{th}$ ray with the solid angle $\Delta\Omega_l$ ($l = 1,...N$) starts from $j_{th}$ boundary element. On each ray equation (7) is integrated over the passed cells to obtain the radiation intensity field:

$$I_{ij}^0 \rightarrow I_{ij}^1 \rightarrow ... \rightarrow I_{ij}^L$$

$$I_{ij}^{m+1} = I_{ij}^m e^{-\sigma_s \Delta s_m} + \frac{\sigma T_i^4}{\pi} (1 - e^{-\sigma_s \Delta s_m})$$

where $L$ is the total number of cell that ray $l$ passed. At boundary cell $j$,

$$I_{ij}^0 = q_j^+/2\pi$$

where $q_j^+$ is the heat flux of the outgoing ray. At boundary cell $i$,

$$q_i^+ = (1 - \epsilon_w) \sum_{l=1}^{N} I_{ij}^l \Delta\Omega_l + \sigma\epsilon_w T_i^4$$

$\epsilon_w$ is the wall emissivity ($\epsilon_w \sim 0.5$). The outgoing heat-flux at the boundary can be recast into an iterative form:

$$q_j^{n+1} = A q_j^n + B$$

where $n$ is the iteration step.

Each outgoing ray is then traced until it hits a solid boundary. During its passage through the medium, the ray losses/gains energy depending on the local composition and temperature of the ambient gas. The accuracy of the DTM depends on the number of the discrete rays and the radiation-grid spacing. Here, we ensure, by successive grid refinements, that the number of rays, and the radiative grid resolution are adequate in our calculations.

3.2 Ray Tracing Technique for General Grids

The key problem remaining is the determination of the relation between a ray and a cell. That is, how to find the set of cells, $Q_m$ ($m = 1,...,L$), passed by the ray $l$. This set of cells is used when computing $\Delta s_m, \sigma_m$ and $T_m$ in the integration sequence (14).

Assume that the cell is so small that each of its surfaces can be approximated by a flat plane. The
The turbulent combustion flow in a gas turbine combustion chamber has been investigated using the above described methods. It is also our aim to study certain aspects of modeling turbulent reacting flows with radiative heat-transfer: the influence of different shapes of presumed PDF on the resulting radiative heat transfer; and the relative importance of radiative heat transfer as compared with other heat-transfer processes (e.g. advective transfer).

4.1 The species concentrations and temperature

The gas turbine combustion chamber has been assumed to be cylindrical and axi-symmetrical. The geometry of the combustors can be seen in the concentration field and temperature field. For convenience, we assume that \( L \) is the length of the combustor in axial direction (\( z \)), \( R \) is the radius of the combustor in inlet plane (i.e., \( x = 0 \)). We use the ratio \( L/R = 4 \).

The combustion chamber includes a liner containing a dilution air entrance and a film-cooling arrangement, as shown in Fig.2-3. The outer wall boundary condition for the energy transfer is assumed to be adiabatic (\( \partial T/\partial n = 0 \)) and the liner wall condition is assumed to be heat conducting in one (normal to the wall) direction. The fuel is Methane, which is injected through the inlet near the central line with inlet velocity of 0.57m/s. The primary air is injected with a velocity of 5.17m/s. The equivalence ratio of the fuel to the primary air is 0.968. The secondary air is supplied at a velocity of 1.015m/s through near side-wall inlets and the liner holes. The overall equivalence ratio is 0.165. The inlet fuel and air are supplied at one atm and 300°K.

The number of grid points used in the calculations is determined by the required accuracy. The accuracy is estimated by solving the problem on several grids with different mesh spacings. In order to keep the grid number minimal without significant loss of accuracy, we use periodic boundary condition in the azimuthal direction based on the observation that the mean steady state flow field is axi-symmetric. The mesh used has 3 grids in the azimuthal direction, 104 grids in the axial direction, and 92 grids in the radial direction. The radiative intensity is calculated on a 3-D grids with number of grids of 53, 47 and 16 in the axial-, radial- and azimuthal direction, respectively. The dependence of the numerical solution on the number of rays can be examined in terms of the temperature field. The
temperature profiles computed by using 16 and 64 rays differ by only 3%. Hence in consequent calculations we use 16 rays emanating from each boundary element.

The iterations are stopped when the residuals of the discretized equations are reduced by five orders of magnitude.

The velocity vector field near the inlets is shown in Fig. 2. The liner guides the secondary air into the main chamber and the dilution channel. This results in a desired temperature field (cf. Fig. 3): low temperature near walls. The recirculation region near the inlets can also be seen in Fig. 2. A consequence of the recirculation is the local high temperature in this region (cf. Fig. 3), which is beneficial for flame stabilization. The upper and lower halves of Fig. 3 show the temperature fields as computed with and without taking the effect of thermal radiation into consideration, respectively. The highest temperatures in these two calculations differ by 200 K (more than 10%). The distribution of the temperature is also quite different: without considering radiation, the high temperature region is located in downstream region across the axis, which is the flame sheet location. In practice, because of the thermal radiation, the high temperature region loses energy, and other cooler regions, especially the low speed flow recirculation region receives energy. The upper half of Fig. 3 shows this effect: the highest temperature is located near the upstream recirculation region, away from the axis of the combustor.

The concentrations of O₂ and CO are shown in Fig. 4. In this case the secondary air stream is fairly strong, so that oxygen is rich near the liner and the combustor wall. The flame is confined in the central region around the combustor axis. CO is also concentrated in this region. The strong secondary stream dilutes the outlet CO concentration. It also delivers sufficient oxygen so that CO is further oxidized to form CO₂.

4.2 Influence of the Shape of the Presumed PDF

In the above calculation the $\delta$ function has been used as the PDF shape for calculation the influence of turbulence on the heat radiation. Namely, the correlation in the mean radiative transfer equation is computed by $\sigma_a T^4 = \sigma_a T^4$. 

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In the following we consider the influence of the shape of the presumed PDF on the radiation calculation, and on the flame temperature distribution. Fig. 5 depicts the profiles of temperature and the radiative source term \((-\nabla \cdot \mathbf{q}_r)\) along the central line of the combustor. The different lines correspond to the different shapes of PDF: the \(\delta\) function; the triangular distribution; the \(\beta\) function with two different levels of temperature fluctuation intensity (10% and 20%). As seen that the radiative source terms are quite sensitive to the shape of the PDF, and also to the selected values of turbulence intensity. It is interesting to note that the \(\beta\)-function distribution gives results close to those of the \(\delta\)-function distribution, especially when the intensity of the temperature fluctuation is small. The triangular distribution gives a radiative heat transfer source term that differs considerably from the results calculated using the other two functions. As a result, the temperature profiles are different for different PDF shapes. The difference of the temperature profiles is smaller compared with the difference of the radiation source terms, due to the combination of other heat transfer effects.

In further calculations the \(\delta\) function is used for simplicity. A more detailed investigation cannot be done without comparison with more accurate data, e.g., data from measurements or from direct calculation of the PDF distribution.

4.3 THE RELATIVE IMPORTANCE OF RADIATION IN HIGH SPEED FLOWS

In the following, we shall investigate the relative importance of the radiative heat transfer in flames with different characteristic velocity scales. The calculation is performed in the same gas turbine combustor geometry as is shown in the previous section. The same grids are employed in this calculation. We keep all the operation conditions the same as before, except the velocity at the inlets. Two cases has been considered. As is shown in Fig. 6, case (a) is the one used in the calculation discussed previously. In case (b), we amplified the inlet flow speed by a factor of ten. That is, the fuel inlet velocity is 5.7 m/s. The primary air velocity is 51.7 m/s. The secondary air is supplied at a velocity of 10.15 m/s.

Fig. 6 depicts the temperature profiles along radial direction at \(x/L = 0.6\) plane (the profiles in other planes have the similar features). As has been discussed earlier, in case (a) the effect of radiation is large. However, the effect of heat radiation in case (b) is negligible, as shown in Fig. 6. This is because that the advective heat transfer is more important in high speed flows,

\[
(-\nabla \cdot \mathbf{q}_r)_{inlet}/(\rho U \kappa)
\]

Figure 5: The temperature profile and the profiles of the radiative source terms \((-\nabla \cdot \mathbf{q}_r)\), normalized at the fuel inlet condition, along the central line of the combustor with different PDF-forms

as is the case for case (b). This supports the assumption of neglecting the radiative heat transfer in some cases, for instance, when asymptotic analysis is used for laminar flamelet [6],[7],[14].

However, in general one should be careful when neglecting the effect of heat radiation. Since in many cases the velocity scales in the field is multiple: there are regions, such as those near stagnation points, where the velocity is generally low, even in high speed inlet flows. Besides, one has to consider other factors interacting with heat radiation: the temperature distributions; the gas, soot or wall absorptivity, emissivity and reflectivity, etc.
5 Concluding Remarks

Calculation of turbulent combustion and radiative heat-transfer in a gas turbine combustion chamber has been carried out. The calculations were based on the generalization of the Discrete Transfer Method for arbitrarily shaped geometries. A ray tracing method is proposed for handling the arbitrary shaped grids.

A less-investigated aspect in turbulent reacting flows is the modeling of the interaction between the temperature fluctuation and the heat radiation. By using different presumed PDF, we found that this aspect may be important in situations where there are large amplitude temperature fluctuations. Using the mean values for computing the radiative source in the energy equation is reasonable in cases with globally low levels of temperature fluctuations.

The calculations reveal that in many cases the radiation heat transfer plays an important role in determining the temperature profiles. The error in the mean temperature may be more than 10% by simply neglecting the effect of radiation. In some other cases, e.g. in high speed flows or low temperature combustion, the relative importance of the heat radiation may be small. However, the error due to the neglect of radiation effect may be large in calculation of other quantities, for instance, the NO$_x$ emissions, soot levels, etc. Thus, it is believed that when one is interested in details, one has to take into account heat radiation.

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References


