In situ adaptive tabulation (ISAT) for combustion chemistry in a network of perfectly stirred reactors (PSRs)

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ABSTRACT

This paper presents an efficient computational implementation of the *in situ* adaptive tabulation (ISAT) approach (Pope, 1997) for combustion chemistry in a network of perfectly stirred reactors (PSRs). A series of PSR calculations is carried out using the direct integration (DI) and ISAT approaches, and validation of DI is performed through comparisons with previous experiments. Assessment of the accuracy of ISAT approach is conducted through direct comparisons with DI calculations. Moreover, accessed region of the composition space, sensitivity of ISAT calculations with respect to the absolute error tolerance values and speedup are analyzed for two different test cases, a hydrogen–air and an ethylene–air combustion case. In summary, the hydrogen–air case resulted in a speedup of 9.8 for 1 million of PSRs in series, whereas for the ethylene–air case it was 42 for 0.3 million PSRs.

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1. Introduction

Accurate predictions of turbulence-chemistry interactions in turbulent reacting flows necessitate a coupled calculation of the flow field and chemical kinetics through a direct integration of the governing equations. However, since the direct integration (DI) of the fundamental equations is extremely compute intensive, some form of averaging and/or modeling is necessary. Modeling turbulent reacting flows using the Reynolds-averaged Navier Stokes (RANS) approach is efficient due to all length scales being modeled. However, in the context of reacting flows, this approach introduces problems with closure of the highly non-linear reaction term. An efficient computation requires the proper choice of a combustion model along with the use of detailed chemical kinetics mechanisms, which could consist of hundreds of species with thousands of chemical reactions. The former can be addressed by treating turbulence-chemistry interactions with the eddy dissipation concept (EDC) (Magnussen and Hjertager, 1981; Magnussen, 1989) or the eddy dissipation model (EDM) (Magnussen and Hjertager, 1977). With regard to the chemistry, significant cost savings can be achieved by resorting to global mechanisms albeit with a reduction in accuracy.

EDM follows the eddy-breakup model (EBM) (Spalding, 1971, 1977), which is primarily based on the assumption of an infinitely fast chemistry and a dominant turbulent mixing time scale. EDC is an extension of the EDM which considers the detailed kinetics by making use of reaction rates obtained from the Arrhenius expressions. The EDC model treats turbulence-chemistry interactions by relating a reactor to the fine structure in turbulence. Reactants are mixed homogeneously within the fine structures which exchange mass and energy with the surrounding fluid. These fine structures of turbulences are treated as perfectly stirred reactors (PSRs). Typical calculations of turbulent flames in gas turbine combustors and furnaces involve computational grids that contain at least a few million cells, and the solution of chemical kinetics equations may be required to advance for thousands of time steps, making the total solution time of the order of a billion. So, it becomes almost computationally infeasible to solve the detailed chemical kinetics for such problems and this makes the *in situ* adaptive tabulation (ISAT) (Pope, 1997), a promising alternative.

ISAT was introduced in Pope (1997), and it is a storage/retrieval method that is primarily dependent on an *in situ* tabulation of the accessed region of the composition space. ISAT has been applied previously to various studies involving – probability density function (PDF) calculations of pairwise mixing stirred reactors (PMSR) (Pope, 1997) – rate controlled constrained manifolds (Tang and Pope, 2002) – unsteady laminar reacting flames (Singer and Pope, 2004; Singer et al., 2006); large eddy simulation (LES) of turbulent flames (Lu et al., 2004) – calculations of turbulent lifted flames

Nomenclature

ρ	density of reacting mixture (kg/m^3)
V	volume of reacting mixture (m^3)
$\dot{m}_{in}$	inlet mass flow rate (kg/s^3)
$\dot{m}_{out}$	outlet mass flow rate (kg/s^3)
Y_i	mass fraction of reacting species, i
$Y_{i,in}$	mass fraction of reacting species, i, at inlet
$Y_{i,int}$	intermediate value of mass fraction of reacting species, i, at inlet
$\dot{\omega}_i^g$	net generation rate of reacting species, i ($kmol/m^3$ s)
MW_i	molecular weight of reacting species, i ($kg/kmol$)
$C_{p,mix}$	specific heat of reacting mixture at constant pressure ($J/kg\,K$)
T	temperature of mixture (K)
P	pressure of mixture (Pa)
$\dot{Q}$	rate of heat transfer from reacting mixture (J/s)
h_i	enthalpy of reacting species, i (J/kg)
$h_{i,in}$	enthalpy of reacting species, i, at inlet (J/kg)
n	total number of reacting species
n_g	total number of gaseous species
n_c	total number of condensed species
τ	residence time of the reactor (s)
ϕ	composition vector
ϕ^0	composition at the initial time, t_0
ϕ^q	query composition

(Gordon et al., 2007) – scaled PDF methods for combustor analysis (James et al., 1999) – computational fluid dynamics (CFD) calculations of nano particle formation by reactive precipitation (Wang and Fox, 2003) – and real time control (Hedengren and Edgar, 2005). In addition, there have also been several developments regarding algorithm improvement and error reduction in ISAT. Performance improvement by modification of the search algorithm (Chen, 2004), analysis of local and global errors in the context of turbulent flames (Liu and Pope, 2005), parallel implementations of ISAT in LES (Lu et al., 2005), improved table searching strategies and error checking and correction algorithms (Lu and Pope, 2009), and extension of the implementation for accelerating the simulation of complex heterogeneous chemical kinetics (Blasi et al., 2016), are some examples of previous works in this area.

The primary objective of the current study is to develop a methodology to incorporate the ISAT approach for *in situ* storage/retrieval of accessed regions in a network of PSRs. PSRs have been used for a few decades now, to study chemical kinetics (Bowman et al., 1973; Marinov and Malte, 1995; Westbrook et al., 1988) and soot formation (North, 2012; Manzello et al., 2007, 2007; Adhikari et al., 2015). They can be considered as idealized experimental environments, which involve species undergoing infinitely fast mixing compared to chemical reactions (Glarborg et al., 1986). In practical systems, the primary zone of a gas turbine combustor has intense recirculation of the gaseous species (Kowalik et al., 1981), and is an example of a PSR.

The performance of ISAT has been tested in the past in the context of what is called a pairwise mixing stirred reactor (PMSR) by Pope (1997). In a PMSR, a certain number of particles is considered with each of them having a specific composition. Outflow, inflow and pairing events occur at discrete times, which ultimately change the composition of each particle. These events occur at different timescales, and thereby the mixing, pairing and residence timescales are involved in the computation. The PMSR computation involves the breakdown of the composition evolution into mixing and reaction fractional steps, and ISAT is only applied to the reaction step. For PSRs on the other hand, the Damkohler number, *Da* is

$\ll 1$, resulting in a chemical timescale much larger than the mixing timescale, and thus the flow is dominated by turbulent mixing. The composition evolution equation of a PSR consists of reaction and mixing steps combined, and the mean residence time represents the overall timescale. As mentioned earlier, the goal here is to test the performance of ISAT in the context of PSRs, and is presented here for the first time. The most relevant study to the current one is Pope (1997), where ISAT was integrated with PMSR. The main difference between the current investigation and Pope (1997) is that unlike Pope (1997), the ISAT is applied to both the mixing and reaction substeps here. In addition, the coupling that is developed here is tested for two different test cases; hydorgen–air combustion and ethylene–air combustion in network of PSRs.

2. ISAT–PSR coupling

This section presents a description of steps involved in the coupling of ISAT with the PSR solution algorithm. The primary issue that is being addressed in this study is a cost-effective solution of PSR equations for a time interval that is known in advance, in the context of a series of PSRs having different thermochemical states, by employing ISAT instead of DI, when possible.

2.1. ISAT–PSR formulation

Consider a steady state PSR consisting of n_g gaseous species and n_c condensed species at any time inside the reactor. The enthalpy of the mixture is h, temperature is T, and the pressure is P. The rate of change of total mass inside the PSR can be related to the mass inflow rate and mass outflow rate as:

$$\frac{d(\rho V)}{dt} = \dot{m}_{in} - \dot{m}_{out} \tag{1}$$

Furthermore, the thermochemical state of the mixture can be represented by ϕ as:

$$\phi = \{Y_1, Y_2, Y_3, \ldots, Y_{n_g}, \ldots, Y_{n_g+n_c}, T, P\}, \tag{2}$$

Since the reaction rates considered are explicitly dependent on temperature, it is desirable to have temperature as one of the dependent variables in lieu of enthalpy, while representing the thermochemical state vector, ϕ, in Eq. (2). A constant pressure reactor is considered here, and Eq. (2) can be re-written as:

$$\phi = \{Y_1, Y_2, Y_3, \ldots, Y_{n_g}, \ldots, Y_{n_g+n_c}, T\} \tag{3}$$

The components of ϕ are changing over time. The evolution of thermochemical state inside the PSR can be represented as:

$$\frac{d\phi_i^0(t)}{dt} = S_i(\phi^0[t]) \tag{4}$$

where $i = 0, 1, 2, \ldots, n_g + n_c$. The term on the right hand side of Eq. (4) is the source term, and it represents the sum of the rate of change of thermochemical composition states due to reaction and transport. Since PSR is a 0-dimensional reactor, there would be no contribution to the source term from transport. However, there is still a contribution from molecular diffusion. As mentioned previously, the mixing timescale in a PSR is extremely high, and turbulent mixing dominates the mixing due to molecular diffusion. With the mean residence time of the PSR, τ is given by,

$$\tau = \frac{\rho V}{\dot{m}_{in}} \tag{5}$$

the equations for species and energy can be written as:

$$\frac{d\phi_i(t)}{dt} = \frac{1}{\tau}(\phi_{i,in} - \phi_i) + \frac{\dot{\omega}_i^g MW_i}{\rho} \tag{6}$$