**ABSTRACT**

Two storage/retrieval schemes have been used to implement detailed chemistry in multidimensional CFD: “*in situ* adaptive tabulation” (ISAT) [1] and “database on-line for function approximation” (DOLFA) [2]. The emphasis is on predicting autoignition in nearly homogeneous to moderately non-homogeneous mixtures (homogeneous-charge compression-ignition engines) and in highly non-homogeneous direct-injection systems (stratified-charge compression-ignition engines). In nearly homogeneous systems, speedups approaching a factor of 100 have been realized compared to direct integration of the chemical source terms; factors of five-to-ten have been obtained in moderately non-homogeneous systems; and smaller – but still significant – speedups have been realized in highly non-homogeneous direct-injection systems. Database size is an important issue in storage/retrieval approaches. Here linear scaling of database size with the number of chemical species has been achieved by limiting the set of independent tabulation variables, while still retaining the full chemical mechanism. Additional strategies to reduce table size have been implemented in DOLFA. With these approaches, it is feasible to use chemical mechanisms involving over 100 species for multidimensional CFD of in-cylinder combustion in IC engines and in other applications.

**INTRODUCTION**

Multidimensional modeling is playing an increasingly important role in the development of next-generation engine combustion systems. Many of the most urgent issues to be addressed require detailed chemical models for hydrocarbon-air oxidation and minor species (pollutant) formation. The requisite chemical mechanisms involve tens-to-hundreds of chemical species and elementary reactions. Examples include autoignition in direct-injection diesel and homogenous-charge compression-ignition (HCCI) engines, and formation/destruction of oxides of nitrogen and other pollutant species. In most cases, it is not practicable to use detailed chemical mechanisms in three-dimensional time-dependent CFD for realistic engine configurations. Key issues include the large number of chemical species and the highly nonlinear, stiff character of the chemical source terms.

Substantial effort has been devoted to the development of strategies to accommodate detailed chemistry in device-scale CFD. Approaches include classic mechanism reduction, automated dimension reduction, storage/retrieval schemes and combinations of these methods. Pope’s *in situ* adaptive tabulation (ISAT) [1] storage/retrieval algorithm provides the foundation for the present work. Compared to alternative tabulation schemes, ISAT offers a number of advantages. First, it is not necessary to pre-compute the reaction table: it is generated on-the-fly (*in situ*) in the course of the CFD calculation. Second, ISAT is *adaptive*; a sensitivity/error
estimation technique is used to establish the region of composition space over which each table entry can be used with specified accuracy. And third, ISAT is efficient; provided that table reuse is sufficiently high, significant speedups can be realized compared to direct integration of the chemical source terms.

ISAT originally was developed in the context of particle-based probability density function (PDF) methods. Applications have been mainly to homogeneous systems and to statistically stationary configurations (e.g., turbulent jet flames) where constant-pressure high-temperature chemistry dominates. In such cases, an asymptotic state corresponding to nearly 100% table retrieves can be reached, and speedups of up to a factor of 1,000 have been reported. Moreover, usage to date generally has been limited to small- to moderate-sized chemical mechanisms (fewer than 50 chemical species). By contrast, the engine autoignition application is non-stationary with time-varying pressure; a typical CFD case corresponds to a single transient combustion event. The number of computational cells used for grid-based CFD is smaller than the number of particles that would be used in a PDF method by at least one order of magnitude. Both low-temperature and high-temperature chemistry must be captured accurately. And mechanisms exceeding 100 chemical species are of interest. For these reasons, it is anticipated that the benefits of ISAT – or of any other storage/retrieval strategy – may be far below those that have been reported in the literature for canonical configurations.

A commercially available implementation of ISAT, ISATAB [3], has been used successfully to model autoignition in nearly homogeneous and moderately non-homogeneous mixtures using n-heptane mechanisms containing up to 160 species [4]. Since that time, the autoignition of highly non-homogeneous systems has been investigated further; and a new storage/retrieval algorithm has been developed (DOLFA [2]) that addresses some of the shortcomings that have been identified in the original ISAT algorithm for this application.

**STORAGE/RETRIEVAL-BASED COMBUSTION CFD**

The underlying finite-volume CFD code solves a system of coupled non-linear partial differential equations (pde’s) for a compressible multi-component chemically reacting mixture [5,6]. Principal pde’s correspond to conservation of mass (continuity), momentum, absolute enthalpy and species mass fractions. An iterative time-implicit segregated pressure-based algorithm patterned after PISO is employed. Turbulence is modeled using a standard two-equation $k$-$\varepsilon$ model; computed dependent variables represent ensemble- (phase-) averaged mean values. The equations are solved on an unstructured deforming mesh with co-located cell-centered variables. Discretization accuracy is first-order in time and up to second-order in space.

Of principal interest here is the implementation of chemical source terms in the species equations. The cell-level end-of-timestep mass fractions $Y(t_0 + \Delta t)$ are computed from the beginning-of-timestep mass fractions $Y^0 = Y(t_0)$ as,

$$Y(t_0 + \Delta t) = Y^0 + \int_{t_0}^{t_0 + \Delta t} S(p(t'), T(t'), Y(t')) dt',$$  \hspace{1cm} (1)

where $S(p, T, Y)$ are the chemical source terms in the species equations. In direct integration, Eq. (1) is solved for each computational cell using a stiff ode solver over the CFD computational timestep.
In a storage/retrieval approach, the end-of-timestep species mass fractions $\overline{Y}(t_0 + \Delta t)$ are tabulated as a function of the beginning-of-timestep mass fractions $\overline{Y}(t_0)$, pressure $p(t_0)$ and temperature $T(t_0)$. Starting from an empty table, the end-of-timestep values required by the CFD code are generated by direct integration (Eq. 1), and the results are stored in a table. In the case of ISAT, a mapping gradient matrix (related to the Jacobian of $\overline{X}$) also is computed and stored; the mapping gradient is used to perform linear interpolation and to establish error bounds. On each subsequent query by the CFD code with new beginning-of-timestep values, one of three actions is taken by ISAT: 1) If the end-of-timestep species mass fractions can be determined to within a prescribed accuracy via linear interpolation from an earlier table entry, then a table look-up and interpolation is performed (a retrieve); 2) If the end-of-timestep mass fractions cannot be determined with sufficient accuracy by linear interpolation from previously tabulated information, then a direct integration is performed and a new table entry is generated (an add). 3) If a direct integration is performed and it is subsequently determined that linear interpolation from a previously tabulated value would, in fact, have sufficed, then the region of accuracy about that previously tabulated value is increased (a grow).

In [4], a reduced set of species mass fractions was employed as independent tabulation variables for ISAT. With this approach, table size increases linearly with the number of chemical species, versus quadratically for the case where all species are retained and the mapping gradient matrix is stored. A robust set of control parameters was identified that yields good performance for ISAT-based CFD of autoignition in nearly homogeneous to moderately non-homogeneous systems (HCCI engines). However, performance was less satisfactory for highly non-homogeneous systems (direct-injection stratified-charge compression-ignition engines).

A NEW DATABASE ALGORITHM: DOLFA

Three characteristics of the baseline ISAT algorithm have been identified that limit its performance in the IC-engine autoignition application, particularly for highly non-homogeneous mixtures. First, ISAT allows for adds and grows, but not for removal and/or restructuring of table entries. The transient nature of the engine combustion process implies that table entries generated early during compression will never be reused later during expansion, for example. Second, the binary tree database structure employed in ISAT can become highly unbalanced and inefficient. And third, the database structure does not guarantee that the table entry closest to a query composition will be located. This can result in the generation of a table entry (an add) in cases where, in principle, a retrieve from a different table entry would have sufficed.

A new algorithm has been developed that addresses these shortcomings: database on-line for function approximation (DOLFA). Key features include a dynamic database where table entries that have not been used recently are deleted periodically and the table restructured, and an algorithm that guarantees that the existing table entry that is closest to a query composition will be found. Details can be found in Ref. [2]. In the following section, results obtained using direct integration, ISAT and DOLFA to model IC engine autoignition are presented and discussed.

AUTOIGNITION IN IC ENGINES

A Nearly Homogeneous Case

The engine configuration is modeled after a diesel engine that has been modified for HCCI operation at Lund University [7]. For HCCI, we focus on a case with a 10.3:1 compression ratio.
at 1,000 r/min and n-heptane fuel at an equivalence ratio of 0.33. The initial composition is uniform while the temperature is non-uniform (fixed wall temperatures); details can be found in Ref. [4]. Computed in-cylinder pressure and temperature traces using direct integration and DOLFA are reproduced in Figure 1; ISAT results are essentially the same as those obtained using DOLFA. Similar levels of agreement are found for all major and minor chemical species.

![Figure 1](image1.png)

**Figure 1.** Computed global in-cylinder pressure (left) and temperature (right) for a nearly homogeneous engine using a 40-species n-heptane mechanism. Direct integration: solid lines; DOLFA: dashed lines.

![Figure 2](image2.png)

**Figure 2.** Left: Cumulative CPU time for ISAT and for DOLFA. Right: Database size for DOLFA using a static database (no deletion of unused entries) versus a dynamic database. Results are for the same nearly homogeneous engine configuration as in Figure 1.

Tabulation performance is summarized in Figure 2. In this case, the CPU time required to form chemical source terms is reduced by more than a factor of 50 with ISAT compared to direct integration; overall CPU time for the entire calculation is reduced by a factor of nine-to-ten. DOLFA CPU time is about 40% lower than that for ISAT. And database size is reduced dramatically in the case where table entries that have not been used recently are discarded and the database is restructured (the “dynamic” case in Figure 2).
A Highly Non-Homogeneous Case

Results for a direct-injection stratified-charge compression-ignition engine are shown in Figures 3 and 4. The engine configuration is similar to the HCCI case considered earlier. Here the compression ratio has been increased to 18.8:1 and gas-phase n-heptane is injected directly into the combustion chamber over a 16-degree duration starting 29 degrees before top-dead center; the global equivalence ratio is approximately 0.45. Initial results reported in Ref. [4] showed poor ISAT performance for this case. Further experimentation with ISAT control parameters has yielded acceptable accuracy compared to direct integration with an approximate break-even in CPU time. However, the ISAT database becomes extremely large. For the case shown in Figure 3, the ISAT database reaches approximately 500 Mb by the end of the run, compared to less than 10 Mb for the dynamic DOLFA algorithm. DOLFA CPU time is approximately 40% less than for ISAT, although ISAT retrieval rates are slightly better (Figure 4).

Figure 3. Computed in-cylinder pressure traces for a highly non-homogeneous case using direct integration, ISAT and DOLFA (left). Evolution of DOLFA database size for a dynamic database case (right).

CONCLUDING REMARKS

Results to date suggest that storage/retrieval offers a viable alternative to direct integration for finite-volume-based CFD in combustion applications. The effectiveness of storage/retrieval increases with increasing spatial homogeneity. However, benefits have been found even in highly non-homogeneous systems. Shortcomings of the baseline ISAT algorithm [1] for the IC engine application have been addressed in a new storage/retrieval algorithm, DOLFA [2].

In the cases reported here, no additional models have been invoked to account for the influence of turbulent fluctuations on mean chemical production rates (turbulence/chemistry interactions). That is, detailed reaction mechanisms have been applied directly using cell-centered mean pressure, temperature and species mass fractions. Turbulence has been shown to influence combustion phasing even in HCCI engines [8,9]. The emphasis here, however, is the numerical implementation of complex chemistry for CFD; an additional correction to account for turbulence/chemistry interactions is expected to have no effect on the salient results of this study. A future direction of this research is to account for turbulence/chemistry interactions using a PDF approach [10].
Figure 4. Cumulative CPU time (left) and retrieval rate (right) for ISAT and DOLFA for the highly non-homogeneous engine configuration of Figure 3.

REFERENCES