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Improved chemical kinetics numerics for the efficient simulation of advanced combustion strategies

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Abstract

The incorporation of detailed chemistry models in internal combustion engine simulations is becoming mandatory as local, globally lean, low-temperature combustion strategies are setting the path towards a more efficient and environmentally sustainable use of energy resources in transportation. In this paper, we assessed the computational efficiency of a recently developed sparse analytical Jacobian chemistry solver, namely 'SpeedCHEM', that features both direct and Krylov-subspace solution methods for maximum efficiency for both small and large mechanism sizes. The code was coupled with a high-dimensional clustering algorithm for grouping homogeneous reactors into clusters with similar states and reactivities, to speed-up the chemical kinetics solution in multidimensional combustion simulations. The methodology was validated within the KIVA-ERC code, and the computational efficiency of both methods was evaluated for different, challenging engine combustion modeling cases, including dual fuel, dual direct-injection and lowload, multiple-injection RCCI, direct injection gasoline compression ignition (GDICI), and HCCI engine operation using semi-detailed chemistry representations. Reaction mechanisms of practical applicability in internal combustion engine CFD simulations were used, ranging from about 50 up to about 200 species. Computational performance for both methods was observed to reduce the computational time for the chemistry solution by up to more than one order of magnitude in comparison to a traditional, dense solution approach, even when employing the same high-efficiency internal sparse algebra and analytical formulations. This confirms that consideration of detailed chemistry is not a bottleneck anymore, allowing use of larger and more refined meshes. Further research that focused on algorithms for fast and efficient advection with a large number of species is suggested.

Introduction

Research for advanced, cleaner and more efficient combustion strategies in internal combustion engines has been guided in the last decade by the advancements in computer modeling. This has enabled understanding of the interactions between fuel-air mixture preparation, ignition kinetics and pollutant formation in both sparkignited and compression ignition combustion modes, through more comprehensive and reliable computer models [1]. Advancements in chemical kinetics modeling have allowed the development of detailed reaction mechanisms for diesel and gasoline fuel surrogates [2-3], that incorporate thousands of species and elementary reaction steps, providing insight into the interactions between hydrocarbon compounds on ignition, and at the same time yielding quantitatively accurate predictions of the major pollutant species – carbon monoxide (CO), unburned hydrocarbons (UHC), nitrogen oxides (NO_x), as well as soot formation precursors (such as polycyclic aromatic hydrocarbons, PAH) [4].

While these models have successfully been applied to simple, zeroor one-dimensional reactor or flame simulations, the computational burden for solving detailed chemical kinetics in multi-dimensional computational fluid dynamics (CFD) simulations is still too demanding when adopting fully comprehensive models. This is due to the stiffness of the system of ODEs describing chemical kinetics, and the expense of advecting a huge number of species over the discretized domain. Thus, current practical solution approaches typically make use of splitting the chemical kinetic system from the CFD solver, and achieve detailed fuel kinetics modeling through:

- Skeletal mechanisms for multiple fuels or multi-component fuel surrogates, with up to about 200 species [5-6]; or local reduction of more detailed reaction mechanisms through on-the-fly reduction methods, often referred to as "dynamic adaptive chemistry" (DAC) methods [7-10]; or direct integration of the detailed mechanisms using advanced, sparse solution numerics [11-13];
- Strategies to reduce the number of chemistry integrations from a full-chemistry approach, that requires solution of a chemical kinetics system on every cell of the CFD domain at every timestep of the flow solver, to a limited number of representative reactor configurations, through storage-retrieval techniques [14-17], multi-zone approaches [18], cell clustering algorithms [19-21].

In this work, we have developed and applied an accurate and computationally efficient methodology to incorporate detailed chemical kinetics in practical internal combustion engine simulations, featuring validated reaction mechanisms for multiple and multi-component fuels. The approach features a sparse analytical Jacobian chemistry solver, with optimal-degree interpolation of expensive thermo-chemistry functions ("SpeedCHEM") [11], to accomplish the integration of the chemical kinetic ODE system, and a high-dimensional clustering algorithm (HDC) [22] to reduce the span of the discretized domain by grouping cells with similar reactivity within a hyper-dimensional state space representation.

The approach was coupled with the KIVA-ERC code, and both the SpeedCHEM solver [23,24] and the HDC clustering algorithm [25] were validated for standard reference cases. The approach was applied and its accuracy and scalability were verified by simulating a variety of engine combustion cases, including dual fuel, dual direct-injection and low-load, multiple-injection RCCI, direct injection gasoline compression ignition with multiple injections (GDICI), direct injection, and HCCI engine operation using a semi-detailed reaction mechanism.

Methodology

Solution of the chemical kinetic ODE system

We developed a computational methodology that features full integration of detailed reaction mechanisms with no mechanism reduction, to provide a numerically exact solution. The SpeedCHEM chemistry program [11] solves the system of ordinary differential equations of chemical kinetics in the form needed in multidimensional CFD codes, and other cases, including constant-volume ignition simulations: given an arbitrary reaction mechanism, containing a set of n_r reactions among n_s species,

$$\sum_{i=1}^{n_s} \nu'_{k,i} M'_i \leftrightarrow \sum_{i=1}^{n_s} \nu''_{k,i} M''_i, \qquad k = 1, \dots, n_r, \tag{1}$$

where v' and v" represent stoichiometric reaction coefficients for reactants and products, respectively, and M the species names, the code computes the laws that determine the temporal evolution of the thermodynamic state of the described homogeneous, reacting gas-phase mixture with species mass conservation, described by:

$$\frac{dY_i}{dt} = \frac{W_i}{\rho} \sum_{k=1}^{n_r} \left(\nu_{k,i}'' - \nu_{k,i}' \right) q_k, \quad i = 1, \dots, n_s,$$
(2)

where the q_k terms represent the reaction rates progress variable, W the species molecular weights, and ρ the mixture density. The equation yields the rates of change of species mass fractions Y_i , that overall verify the mass conservation constraint: $\Sigma Y_i = 1$, or $\Sigma dY_i/dt = 0$. Energy conservation, for ignition in a constant-volume adiabatic reactor, is given by:

$$\frac{dT}{dt} = -\frac{1}{\overline{c}_{v}} \sum_{i=1}^{n_{s}} \left(\frac{U_{i}}{W_{i}} \frac{dY_{i}}{dt} \right), \tag{3}$$

where U represents the species' molar internal energies, \overline{C}_v the mixture average specific heat at constant volume in mass units, and the ODE yields the rate of change of reactor temperature, dT/dt.

Libraries for the evaluation of species and mixture-averaged thermodynamic properties and of the kinetic laws for different reaction types (Arrhenius, three-body, etc.) are included in the code. All of the equations are calculated in a matrix-based representation that makes use of an internal sparse matrix algebra library, specifically developed for this application. As Jacobian matrix evaluation and solution are the most demanding tasks during the integration of the ODE system [11,26] due to its stiff and sparse nature. Solution of the chemical kinetics problem is accomplished by integrating the system of equations with a number of computationally efficient stiff-ODE solvers, including VODE, LSODE, DASSL, RADAU5, RODAS, and MEBDF. Where not available, the internal ODE's sparse algebra for each of these solvers was extended with the capability for solving linear systems using sparse matrices and direct sparse factorization through LU decomposition. Furthermore, an optimal-degree interpolation approach for computationally expensive temperature-dependent thermodynamic functions and reaction rate parameters allowed their evaluation to be sped up by up to two orders of magnitude in comparison with their evaluation using intrinsic compiler functions [25].

The major advantage of this computational setup is that a numerically accurate solution can be provided in an overall CPU time that scales linearly with the number of species, as reported in Figure 1 for constant-volume ignition cases. The overall computational performance was tested for an ignition delay study on a range of

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reaction mechanisms for single and multi-component hydrocarbon fuels. The tests featured 18 ignition delay calculations at stoichiometric conditions, initial pressure of 20 bar, initial temperatures between 700K and 1400K, and integration tolerances of $\epsilon_R = 10^{-8}, \, \epsilon_A = 10^{-20}$, on an Intel Core i5-2400 personal computer running at 3100 MHz and with 8GB DDR3 memory with 1333 MHz frequency.



Figure 1 - Linear scalability of the SpeedCHEM solver for ignition delay calculations. (black) dense, (blue) sparse, (red) Krylov linear system solver comparison.

It was observed that, for the ignition delay calculations, the SpeedCHEM solver ran from about 2 up to about 7 times faster than what has been reported for other sparse chemistry solvers [12] for the range of mechanism sizes of interest to CFD simulations, i.e., $50 < n_s < 700$.

When large reaction mechanisms are used, the direct solution of Jacobian-associated linear systems through sparse LU decomposition as in the aforementioned solvers may be expensive. Thus, preconditioning capabilities were implemented in the solver to enable coupling with iterative Krylov subspace solvers, such as the GMRES algorithm implemented in LSODKR, VODPK, DASKR. A full study of the derivation and calibration of a suitable preconditioner is reported in [26]; however, it was shown, as also summarized in Figure 1, that using the direct solver was the optimum approach for the range of mechanism sizes applicable to CFD simulations. Significant CPU time savings were enabled by the Krylov solver only for extremely large reaction mechanisms ($n_s > 7000$).

High-dimensional cell clustering (HDC)

Even with the computational speed-ups allowed by the SpeedCHEM package, the full chemistry solution in engine CFD simulations is still inefficient due to its inability to identify regions in the domain with similar reactivities, and thus to reduce the number of reactor calculations at every time-step of the fluid solver. Turbulence-chemistry interaction models have been developed to account for the detailed chemistry at the cell level. However, the neglect of sub-grid scale effects, and the use of direct chemistry integration has been shown to provide good results for both conventional diesel and low-temperature combustion [27], even on coarse grids. This enables the possibility of adopting a clustering approach that groups cells based on their thermo-chemical state.

The approach adopted in this study is reported in Figure 2: 1) First, a suitable cell clustering algorithm is used to identify cells in the discretized domain with similar thermodynamic states and reactivities; 2) then, the cells are 'grouped', or 'clustered', into larger homogeneous adiabatic reactors based on a mass weighting approach; 3) the chemistry ODE system is integrated only for this smaller set of 'cell clusters', providing rates of change of species mass fractions for each in the current CFD solver time step; 4) finally, the rates of change in species mass fractions are re-mapped back to the individual cells, using a mass-conservation based approach.



Figure 2 - Schematic of the CFD chemistry solution approach with cell clustering.

In the present study, SpeedCHEM was used as the chemistry solver, and the procedure developed by Babajimopoulos et al. [18] and improved by Liang et al. [28] was adopted for remapping. A high-dimensional clustering algorithm [22] was developed and used to accomplish for cell clustering.

The developed algorithm considers the chemical states of each cell in the domain, viz., temperature and selected species mass fractions, to define a high-dimensional representation of the initial reactor conditions, \mathbf{x}_j , $j = 1, ..., n_{cells}$, where the total number of dimensions d is given by temperature plus a selected subset of species S:

$$\begin{aligned} x_{1,j} &= T_j, \\ x_{2:d,j} &= Y_{k,j}, \forall k \in \mathbf{S}. \end{aligned}$$

$$\tag{4}$$

In order to reduce the variable dependency of the results, the algorithm operates in a purely geometrical hyper-space, where each cell's variable is normalized within its current global, in-cylinder range. Thus, the HDC algorithm needs to accomplish the task of clustering a cloud of points in a high-dimensional hyperspace.

To provide the algorithm with the required accuracy for combustion calculations, the following strategies were adopted:

- The distance measure should not mitigate distances among each single dimension, as every variable in the high-dimensional representation has a different physical meaning; thus, the 'Manhattan' distance metrics were adopted, as represented in Figure 3, which express the distance function *d* between two arbitrary points **x** and **y** in the high-dimensional space as:

$$d_M(\mathbf{x}, \mathbf{y}) = \sum_{i=1}^d |x_i - y_i|.$$
⁽⁵⁾

- The user needs to provide temperature and mass fraction accuracies that should not be exceeded by the algorithm. Thus, it was chosen to initialize the clustering procedure with an initial set of cluster centers, placed in a grid-like fashion (also extremely efficient as it is possible to assign each cluster center a fast unique index as in block-structured grids), as reported in Figure 4. Some of the clusters may be deleted when they are not boxing any points; the initial distances among the cluster centers being defined by the accuracy constraints in the physical (dimensional) space;
- The cluster centers should not move further than the requested accuracy distances during the execution of the clustering algorithm, otherwise the accuracy settings would not be complied with. Thus, a "bounding-box" constraint was defined, i.e., that every cluster center could only have as member points, any of the ones initially placed in the neighboring 'boxes'.

These considerations led to the development of a modified version of the widely adopted k-means algorithm [29] into a 'bounding-boxconstrained k-means', or BBC-kmeans [22]. The algorithm proceeds similarly as the k-means algorithm, i.e., at every iteration, the clustered partition is improved by updating the cluster center positions as the geometrical averages of their member points' positions, and then re-evaluating all the point-to-cluster distances to assign every point to the closest cluster center (whose position has changed from the previous iteration). The grid-like discretization and boxing constraints improve the general k-means approach by 1) establishing a physically correct cluster center initialization; 2) complying with the desired accuracy constraints in the physical domain; 3) reduce the algorithm's computational cost from $O(n_p n_c)$, where n_p is the number of points and n_c the number of clusters, to $O(n_p 2^d)$, where d is the current number of dimensions, as every point is compared only to its boxing cluster centers, and not to all of them anymore. This dramatically affects the algorithm's performance in practical cases, where point-to-cluster distance calculations represent the bottleneck to the algorithm's scaling. Another important feature of the adopted approach is that the number of cluster centers, and thus the overall speed-up of the chemistry integration procedure, is automatically determined by the number of dimensions and the accuracy constraints only, and not on the number of points to be grouped.

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Figure 3 - Comparison between Euclidean (blue) and 'Manhattan' (red) distance measures, in a two-dimensional space.



Figure 4 - Example of operation of the HDC algorithm over a 2D dataset. The benchmark points set is colored according to final cluster membership. Red circles indicate initial cluster center positions, yellow stars with black lines the final cluster centers positions, and

An overview of the mechanics of the present approach is reported in Figure 4 for a sample 2D benchmark featuring 15 well-defined point clouds [30], and where the clustering algorithm is initialized to 20 initial cluster centers. The initial cluster grid-like discretization has red circles and lines, while the final cluster centers are yellow stars and black lines.

Engine Simulation Results

conserved grid-like structure.

Computational setup

The developed computational approach was tested for a range of engine simulation problems, featuring very different combustion regimes and engine operation modes. All of the simulations were run using the KIVA-ERC code [31], a customized version of the KIVA-3v code with improved sub-models for spray dynamics and vaporization, turbulence and wall heat transfer treatments. The original detailed chemistry capability was replaced by the current SpeedCHEM solver and the high-dimensional clustering algorithm implementation. Details of the sub-models are reported in Table 1. The HDC clustering algorithm setup is reported in Table 2. A temperature resolution of 10 K and a species mass fraction resolution of 100 ppm (mass) was used for the cluster center initialization. As a high-dimensional state space representation, temperature and a subset of species including O2, HO2, CO2, H2O, as well as all the fuel components, were used. The impact of temperature and species resolution, as well as of the species subset, on the computational accuracy and efficiency of the approach were studied in [22].

Table 1 - Sub-models in the KIVA-ERC code for the engine simulations in the present paper.

Phenomenon	Sub-model	
Spray breakup	KH-RT instability, Beale and Reitz [32]	
Near-nozzle flow	Gas-jet theory, Abani et al. [33]	
Droplet collision	O'Rourke model [34] with ROI (radius-of-influence), [33]	
Wall film	O'Rourke and Amsden [34]	
Evaporation	Discrete multi-component, Ra and Reitz [35]	
Turbulence	RNG k- ε, Han and Reitz [36]	
Combustion	SpeedCHEM, Perini et al. [11,23]	
Chemistry grouping	HDC algorithm, Perini et al. [22,25]	

Table 2–Common HDC parameters settings for the cases presented in this study.

Parameter	Value	
Fuel species set	$\begin{array}{l} -nC_{7}H_{16}, iC_{8}H_{18}(PRF) \\ -nC_{7}H_{16}, iC_{10}H_{22}, iC_{16}H_{34}, nC_{16}H_{34}, \\ C_{18}H_{38}, C_{21}H_{44}(multiChem) \end{array}$	
Other included species	O ₂ , HO ₂ , CO ₂ , H ₂ O	
Distance measure	Manhattan	
Temperature resolution and span	$\varepsilon_{\rm T} = 10.0$ K, $\sigma_{\rm T} = 1000$	
Species mass fraction resolution and span	$\epsilon_{\rm Y}=10^{-4},\sigma_{\rm Y}=4$	

Here it was found that temperature has the greatest impact, and that using stricter tolerances, like 5 K, is not worth as the accuracy improvement is not justified by the corresponding increase in CPU time. Furthermore it was seen that the species resolution has a smaller impact, as species quantities span orders of magnitude and typically the maximum species span, of 4 points for each species dimension, is always reached.

2D, HCCI combustion with Primary Reference Fuels

2D HCCI combustion cases in the light-duty GM 1.9L diesel engine were modeled following the experiments by Dempsey et al. [37]. A skeletal PRF-PAH mechanism with 108 species and 542 reactions [38], obtained by reducing the detailed LLNL mechanism by Mehl et al. [39], and originally developed to model detailed soot formation kinetics, was used.



Figure 5 - Predicted 2D HCCI pressure and heat release traces with full chemistry (solid) or HDC (dashed+marks).



Figure 6 - Predicted 2D HCCI pollutant emissions (UHC and NO_x) with full chemistry (solid) or HDC (dashed+marks).

A two-dimensional computational grid featuring 550 cells at BDC, was used, with modification to the KIVA grid snapper to allow for at least 10 cell layers to be kept in the squish region when the piston is near top dead centre (TDC). Predicted in-cylinder pressure results are plotted in Figure 5 for two cases with different PRF fuel compositions and intake temperatures. An experimental vs. numerical validation of the reaction mechanism can be found in [38].

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Very small differences can be noticed in the predicted pressure traces when using the full chemistry approach or the clustering algorithm. It should be noted that very good agreement was observed also in terms of pollutant emission predictions, such as the unburned hydrocarbons and nitrogen oxides shown in Figure 6. Here, good agreement is shown despite the different orders of magnitude spanned, providing noticeably greater accuracy than other cell clustering approaches, where differences in species concentrations are reported to be up to a factor of two at the end of the simulation [17].



Figure 7 - Predicted pressure and heat release traces in the RCCI SCOTE engine.

Finally, the CPU time performance showed a consistent reduction across the cases of slightly more than 4 times, from about 35 minutes to 8.5 minutes, with a maximum integration time-step of the CFD solver of 10 μ s. The same analysis was repeated with a much more refined grid having a spatial resolution of 0.7 mm, and featuring 3060 cells at BDC, and yielded similar results with a speed-up factor of 5.7 times. It should be noted that the CPU times reported are referred to a single CPU serial run. These result point out that this advanced chemistry solution approach enables HCCI simulations with accurate heat transfer modeling to be carried out in CPU times similar to those of much more simplified reactor-network-based multi-zone models.

Heavy Duty, Dual-Fuel Direct Injection RCCI

The second test case featured heavy-duty, dual-fuel RCCI combustion achieved with direct injection of n-heptane and iso-octane primary reference fuels with two injectors in the Caterpillar SCOTE engine, modified with an RCCI piston. 9bar IMEP at 1300 rev/min was achieved through 62.1 mg premixed iso-octane, 20.7 mg injected iso-octane at 100 degrees bTDC and 600 bar injection pressure; then, 10.2 mg n-heptane were injected at 100 bar in two steps, 58 and 37 degrees bTDC using a 2/3 vs. 1/3 ratio. The case is based on the experimental measurements by Wissink et al. [40]. A full 360-degree mesh of the combustion chamber was used for the simulations, due to non-axial placement of the injectors, with about 49k cells at bottom dead center. Combustion chemistry was simulated using the ERC PRF mechanism by Ra and Reitz [5].

As Figure 7 shows, the HDC algorithm provided good match of the in-cylinder pressure and heat release traces even in this very challenging case, where three injections produce the premixed fuelair mixture. Negligible errors in terms of the performance and pollutant parameters were observed, as reported in detail in Table 3, and locally in-cylinder in Figure 8.

In order to test the scaling of the computational times with the HDC algorithm for more refined grid resolutions, typical of full multidimensional simulations, two more refined grids were generated by applying a uniform refinement factor in every dimension, having about 86k and 262k cells at BDC, respectively. A representation of the grids is reported in Figure 9. Comparison between predicted results when using either the full chemistry or the HDC approach in Table 3 show that, as expected, the accuracy of the clustering algorithm is not affected by the number of cells in the domain, as the clustering procedure is bound to the user's temperature and species mass fraction constraints of Table 2. From the point of view of CPU time, as also reported in Figure 10, significant savings, always greater than 90% were seen for the chemistry part of the calculations. For all the grids tested, the amount of time spent on chemistry was less than 10% of the total CPU time, confirming the present chemistry approach allows more refined and accurate grids to be used for practical simulations.

Low-load Gasoline Compression Ignition Combustion

GDICI combustion in a light-duty, compression ignition engine was studied using 75 RON (74 AKI/PRF) and 93 RON (87 AKI/PRF) gasoline fuels, adopting a triple injection strategy. 75 RON fuel was used to produce 2 bar BMEP load at 1500



Figure 8 - (left) Full chemistry vs. (right) HDC comparison at different crank angle. -80 to -30 CA: equivalence ratios; -8 to 130 CA: temperature.

rev/min and 5 bar BMEP load at 2000 rev/min, whereas 93 RON fuel was used to investigate 5 bar BMEP load condition only, as it was difficult to achieve a lower load with 93 RON gasoline due to its poor auto-ignition characteristics. The cases mimic the experiments by Ciatti et al. [41] in the study by Adhikary et al. [42].

Table 3 - Engine-out performance parameters for the RCCI SCOTE engine case. Grid resolution study.

49k cells

	full chem.	HDC	diff. [%]
Chemistry CPU time [h]	38.6	1.47	-96.2
ISFC [g/kWh]	163.4	163.5	-0.06
Comb. Efficiency [%]	98.2	98.1	-0.10
CA50 [deg ATDC]	6.50	6.52	0.31
Soot [g/kg _f]	8.80e-2	9.12e-2	3.63
NOx [g/kg _f]	8.00e-2	7.01e-2	12.3
HC [g/kg _f]	14.8	15.7	6.08
CO [g/kg _f]	6.65	6.17	-7.21

86k cells

	full chem.	HDC	diff. [%]
Chemistry CPU time [h]	71.7	2.48	-96.5
ISFC [g/kWh]	163.1	163.2	0.06
Comb. Efficiency [%]	98.2	98.1	-0.10
CA50 [deg ATDC]	6.52	6.51	-0.15
Soot [g/kg _f]	8.48e-2	8.86e-2	4.48
NOx [g/kg _f]	8.10e-2	6.21e-2	-23.3
HC [g/kg _f]	14.7	16.1	9.52
CO [g/kg _f]	6.31	6.13	-2.85

262k cells

	full chem.	HDC	diff. [%]
Chemistry CPU time [h]	320.5	12.8	-96.0
ISFC [g/kWh]	162.8	163.0	0.12
Comb. Efficiency [%]	98.2	98.0	-0.20
CA50 [deg ATDC]	6.52	6.51	-0.15
Soot [g/kg _f]	8.25e-2	8.60e-2	4.24
NOx [g/kg _f]	7.70e-2	4.84e-2	-37.1
HC [g/kg _f]	15.6	17.9	14.7
CO [g/kg _f]	6.27	5.87	-6.38

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Figure 9 - Cross-sectional view of the computational grids used for the RCCI calculations.



Figure 10 - Simulation CPU times for the RCCI case, with different grid resolutions. Left bar: full chemistry; right bar: HDC.



Figure 11 - Pressure trace comparison for four low-load GDICI simulations with variable load, PRF number and EGR. (solid) full chemistry, (dashed+marks) HDC.



Figure 12 - CPU time comparison for the four GDICI cases. (left) full chemistry, (right) HDC.

The study used a computational mesh representing an engine sector and made of 8100 cells at BDC, and the ERC PRF mechanism [5] was used to simulate combustion of the variable RON gasoline surrogate. more details on the modeling approach validation can be found in [42]. A significant speed-up of 26.3 times was observed in terms of overall chemistry solution time when using the HDC algorithm on the full mesh, so that the total simulation time could be reduced from 58 h to 20.5 h when running on a single CPU, as reported in Figure 10.

Performance of the proposed methodology is reported in Figure 11 and Figure 12. Here, the computational accuracy was seen at the whole range of loads, fuel PRF numbers and EGR content simulated, and in presence of complex spray-flow interactions given by the triple injection strategy. Overall computational times for chemistry could be reduced by 10.3 times in the average, allowing simulations with an 11k-cells grid to be computed in up to less than one hour on a single CPU.

A summary of predicted main combustion parameters and engine-out emissions for the GDICI cases is finally reported in Table 4. The results show excellent agreement in combustion timing (CA50), where the largest error when using clustering adds up to 0.04% in comparison with the full chemistry approach; the overall good accuracy of the combustion development prediction is also confirmed by the low discrepancies in total heat release or combustion efficiency, not larger than 0.53%. Also specific fuel consumption, whose measure includes an estimate of how much accurately the incylinder pressure and wall heat transfer have been calculated throughout the simulation, is predicted using clustering well within a 1% error in comparison with the full chemistry approach.

As far as the major pollutants are concerned, a more than reasonable accuracy is seen for all of the components, as errors in the range between 1 to 10% are seen. Only a single error value pops up, corresponding to NO_x prediction error in the very low load and high EGR case, which added up to about 35%.

Table 4 - Engine-out performance parameters for the low-loadGasoline Compression Ignition cases.

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	full chem.	HDC	diff. [%]
Chemistry CPU [h]	2.83	0.21	-92.6
ISFC [g/kWh]	202.7	203.5	0.44
Tot. heat release [J]	361	359	-0.53
CA50 [deg ATDC]	8.01	8.01	0.03
Soot [g/kg _f]	3.97e-4	4.09e-4	3.10
NOx [g/kg _f]	2.05	1.27	-37.6
HC [g/kg _f]	65.6	69.2	5.53
CO [g/kg _f]	83.5	88.8	6.4

5 bar IMEP, PRF74, 27% EGR

	full chem.	HDC	diff. [%]
Chemistry CPU [h]	3.40	0.43	-87.4
ISFC [g/kWh]	193.6	191.8	-0.92
Tot. heat release [J]	639.4	640.1	0.12
CA50 [deg ATDC]	8.02	8.02	0.04
Soot [g/kg _f]	2.80e-1	2.78e-1	-0.68
NOx [g/kg _f]	8.53	8.88	4.11
HC [g/kg _f]	15.2	15.2	-0.14
CO [g/kg _f]	47.6	41.9	-11.9

5 bar IMEP, PRF87, 6% EGR

	full chem.	HDC	diff. [%]
Chemistry CPU [h]	3.16	0.38	-88.0
ISFC [g/kWh]	190.7	189.4	-0.66
Tot. heat release [J]	778.0	777.2	-0.11
CA50 [deg ATDC]	7.01	7.01	0.04
Soot [g/kg _f]	1.74e-1	1.65e-1	-5.54
NOx [g/kg _f]	9.70	9.80	1.01
HC [g/kg _f]	12.7	13.3	4.62
CO [g/kg _f]	38.2	38.1	-0.31

This points out for possible improvements in clustering/remapping procedure to be identified especially in: 1) the adopted remapping procedure by Liang et al. [9] conserves mass but not elements; this may have an impact in terms of undesired accumulation of non-negligible quantities in the species whose mass fractions are small, negligible for combustion timing but that can have an impact on pollutant formation. 2) the heat-capacity-based cluster temperature evaluation guarantees results within the user temperature resolution, but could be improved by a more accurate, yet computationally intensive, internal-energy-based iterative procedure.

Realistic surrogate fuel modeling

Achieving composition-wise comprehensive fuel modeling is essential to improve combustion process simulation and emission analysis, especially for advanced engine development strategies, such as low temperature combustion and direct injection, and for complex alternative diesel fuels. At the same time, a multi-component fuel chemistry model approach both requires a comprehensive fuel drop physical representation, and multiple reaction pathways modeling, that leads to having a large, computationally expensive reaction mechanism which would be impossible to simulate with a dense chemistry approach. In the current study, F-76 fuel spray combustion in a constant volume chamber is simulated using a 21-component physical fuel surrogate model for spray modeling, coupled with a multiChem reaction mechanism featuring 225 species and 1087 reactions [44]. The components in the 21-component fuel model were carefully chosen to represent major species found in an experimental speciation data [45] for the fuel and the model fuel composition was formulated to describe the fuel's physical properties by matching its distillation profile, specific gravity, lower heating value, hydrogen-tocarbon (H/C) ratio and chemical class contents with measured data. The reaction mechanism was developed to consider each of the 21components in the chemistry calculation using the PSGCR model [44] that employs either generic or detailed reaction pathways.

The test-case used for the validation of the HDC algorithm, in presence of multi-component spray vaporization and combustion, features a single-pulse injection from a 7-hole common-rail injector, an injection duration of about 2.4 ms and a total injected mass of about 103 mg.



Figure 13 - Predicted pressure and heat release rate comparison for the realistic diesel surrogate constant volume combustion case. Full chemistry (dashed black line + marks) vs. HDC solutions (colored solid lines) with a different number of mandatory fuel components, n_{fr} for the clustering procedure.

Diesel spray is injected in a high-temperature and high-pressure environment, whose initial conditions of 32 bar pressure and about 800 K temperature, are experimentally achieved after spark ignition of an acetylene/oxygen/nitrogen premixed charge. The CFD model features a sector mesh representing a single nozzle hole and one seventh of the cylindrical combustion vessel, with 8.6k cells. Full details on the detailed fuel composition, and on the experimental conditions for this test case can be found in [44].



Figure 14 - Predicted local temperature and species mass fractions at a vertical plane containing the injection axis, 4.0 ms after the start of injection. (left) Full chemistry vs. (right) HDC, $n_f = 4$.

As far as the HDC clustering algorithm performance was concerned, a species subset study was established in order to understand which are the effects of using a larger number of chemical components in the high-dimensional representation. In particular, a subset of the 21 representative fuel components, made up of the 3 to 6 largest ones in terms of initial mass fraction, as reported in Table 2 ("multiChem"), was always mandatorily included in the clustering procedure, while all of the remaining components were only dynamically included. According to our assumption, at runtime, at the beginning of every call to the clustering procedure, a non-mandatory fuel component could be flagged as 'active' and actually included in the clustering

procedure if and only if its average mass fraction in the whole domain exceeded a user-defined threshold, set at $Y_{min}=0.005.$

In Figures 13 to 15 the results after the species subset study, considering a number of mandatory largest fuel components $n_f = 3, 4, 5, 6$, are presented. First, in Figure 13, the results in terms of overall predicted pressure and heat release rate trace are presented, and compared to the full chemistry approach. All of the species subsets yield extremely accurate ignition timing. However, when using the largest species sets, i.e., $n_f = 5, 6$, predicted ignition timing appears to be delayed by about 0.04 ms than when using the full chemistry approach. A vertical cross-sectional slice of the constant volume chamber, intersecting the injection axis for one of the nozzles, is reported in Figure 14. The plots show that the results, when adopting the clustering algorithm, are locally consistent with the full chemistry approach, i.e. the methodology is able to capture not only average combustion timing, but local composition and thermodynamics.

A study of the error introduced by the clustering procedure on the multi-component fuel surrogate case is reported in Figure 15. Here, an error norm definition according to [22] was used:



Figure 15 - Clustering error and CPU time comparison for the realistic diesel surrogate case vs. number of mandatory fuel components, n_{fr} for the clustering procedure.



Figure 16 - CPU time comparison for the realistic diesel surrogate case. Full chemistry vs. HDC solutions with a different number of mandatory fuel components, n_6 for the clustering procedure.

Equation (6) represents the average cumulative relative error of the clustered solutions over predicted global temperature and pressure. From Figure 15, it appears that the optimal solution from an error point of view was the one that featured $n_f = 4$ mandatory fuel components, whose error was anyway only slightly different from the $n_f = 3$ solution.

The overall CPU time increased noticeably when using larger numbers of mandatory fuel components, even if it was still significantly smaller than the CPU time required by the full chemistry approach. It should be noted that, even if the overall error for larger numbers of mandatory components was larger, it was still within acceptable error limits, as the predicted overall ignition timing was delayed by only about 0.04 ms, or 1.5%, in comparison with the full chemistry case.

Figure 16 finally shows the amount of speed-up allowed on the chemistry solution by the clustering procedure: it ranged from about 2.7 times in the worst case, where $n_f = 6$, up to about 3.7 times where $n_f = 3$.

Conclusions

A methodology for the computationally efficient incorporation of detailed chemical kinetics mechanisms in internal combustion engine simulations of advanced combustion strategies with multiple and multi-component fuels was developed. The methodology features the adoption of a sparse analytical Jacobian chemistry solver (SpeedCHEM) and of a high-dimensional cell clustering (HDC) algorithm. The computational performance of the sparse solver achieved up to three orders of magnitude speed-up in comparison with the traditional, dense chemistry approach, for large mechanisms of up to about 7000 species, enabling engine CFD simulations to be run efficiently even with semi-detailed reaction mechanisms with hundreds of species. The clustering algorithm performance was validated against the full chemistry approach for a range of challenging engine combustion modes, including HCCI, dual-fuel, dual-direct injector RCCI at high load, gasoline compression ignition (GDICI), and constant-volume spray combustion with realistic fuel surrogate modeling. The following conclusions were drawn:

- The sparse analytical Jacobian chemistry solver enables CFD simulations with comprehensive mechanisms to be practically viable, through reducing the computational burden by up to three orders of magnitude in comparison with the traditional dense approach, and with no ad hoc simplifications in the chemistry mechanism;
- The HDC algorithm overcame the limitations of current clustering algorithms, whose efficiency deteriorates on large grids and in presence of multi-component fuels. A grid-independent and unsupervised clustering procedure was used that is only bound to definite accuracy constraints for temperature and species mass fractions;
- The methodology was successfully applied fora variety of advanced combustion strategies cases, where the range of thermo-chemical conditions is so broad that chemistry simplification algorithms are typically extremely inaccurate, or computationally inefficient;
- For HCCI combustion, the multi-dimensional modeling approach is competitive with simplified multi-zone modeling, as full chemistry, coupled with detailed transport and heat transfer can be modeled in similar CPU times;
- The approach allowed reduction of the CPU time spent on chemistry by up to about 30 times, with differences in predicted engine output from the full approach being smaller than other published approaches. The largest deviations were seen in NO_x predictions, that however already showed significant grid dependency.
- Practical simulations with detailed chemistry and geometry modeling can now be effectively accomplished.

The present results have demonstrated that the computational burden due to combustion kinetics can be reduced not to be a bottleneck in the overall simulation framework by the adoption of advanced combustion simulation algorithms. This suggests for further research to focus on enabling engine simulations to be run with comprehensive reaction mechanisms that feature up to thousands species, through studying appropriate numerics for fluid transport when a very large number of species is present.

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