

# Multi-timescale and Correlated Dynamic Adaptive Chemistry and Transport (CO-DACT) Modeling of Ignition and Flame Propagation of Jet Fuel Surrogate Mixtures

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**Abstract**—A correlated dynamic adaptive chemistry and transport (CO-DACT) method is developed based on our previous correlated dynamic adaptive chemistry (CO-DAC) method to further improve the computational efficiency of the transport coefficients such as the mass diffusivities, heat conductivities, and viscosities. The concept of the correlated groups in both time and space coordinates for chemistry and transport is proposed by using a few key phase parameters which dominate the chemistry pathways and transport coefficients. Correlated reduced chemistry and transport coefficients are updated dynamically by specifying different threshold values of phase parameters of correlated groups. For transport, the mixture averaged diffusion model is applied to calculate the transport coefficients based on the correlated groups. Only one calculation of the transport coefficients is required for all the computation cells in the same correlated group. The advantages of the CO-DACT method are that it not only provides the flexibility and accuracy for the calculation of chemistry and transport coefficients for a large kinetic mechanism but also avoids redundant calculations in time and space when the chemistry pathways and the transport coefficients are correlated due to the similarities in phase space. The simulations of premixed propagating spherical flames as well as one-dimensional diffusion flames of a jet surrogate fuel are carried out to validate the proposed algorithm. The impact of the selection of the phase parameters as well as the influence of the threshold value at various pressures and equivalent ratios will be examined in this paper. The results show that the present CO-DACT method is not only computationally efficient (faster by two-orders of magnitudes) but also robust and accurate for large kinetic mechanisms.

## I. INTRODUCTION

On the fly model reduction and calculations of transport properties for a large kinetic mechanism on every computational grid and time step are computationally expensive. Recognizing that similar reaction pathways and transport processes often occur repetitively at different locations and time steps in the entire computation domain, we propose a correlated dynamic adaptive chemistry and transport (CO-DACT) model reduction method to drastically improve the computation efficiency by introducing a concept of the correlated reaction pathways and transport processes and avoiding redundant calculations of model reduction and transport properties in the entire computation domain.

## II. METHOD AND RESULTS

The basic idea of the CO-DACT method is schematically shown in Figure 1. The time and space correlations of reaction pathways and transport processes are examined between different time steps and computation cells by using a pre-specified phase parameter set. If the variation of the phase parameters are within a small threshold, a single reduced reaction model and one set of linearly extrapolated transport properties will be used for all correlated cells. Otherwise, a new reduced reaction model and transport property set will be locally generated.

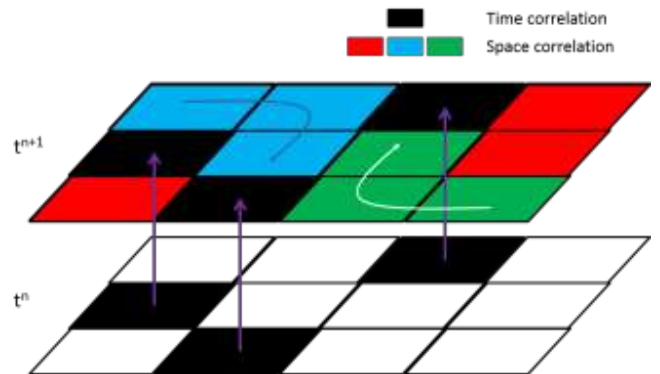


Fig. 1 Schematic of time and space correlations in chemistry and transport. Black cells are time correlation groups and red, blue and green cells are space correlation groups.

The CO-DACT method is integrated with hybrid multi-timescale (HMTS) method for efficient chemistry integration. The resulting HMTS/CO-DACT method is compared with HMTS and HMTS/DAC [1], respectively, for calculating ignition and a premixed spherical propagating flame with a jet fuel surrogate model (with 425 species and 2275 reactions) [2].

The premixed spherical flame is ignited at the center of the domain by a hot spot with 2000 K and 2 mm radius. The initial temperature, pressure and equivalence ratio of the homogeneous jet fuel surrogate mixture are 300 K, 10 atm and 1.0, respectively. The domain size is 5 cm with

transmissive outer boundary condition. Figure 2 shows the time-dependent outwardly propagating spherical flame trajectories calculated by CO-DAC method and CO-DACT method. It is seen that the present CO-DACT method shows excellent agreement compared with the CO-DAC method. The largest relative error in flame trajectory is less than 0.5%, which is far below the experimental accuracy of flame speed measurements.

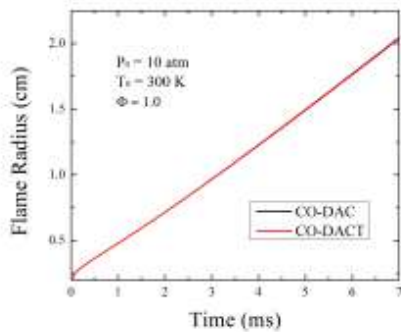


Fig. 2 Flame trajectories of stoichiometric jet fuel surrogate mixture at 10 atm and 300 K.

Figure 3 shows the predicted flame structure of the temperature and major species of the spherical flame at the physical flame propagation time of  $t = 4$  ms. The distributions of temperature and major species  $O_2$  and  $H_2O$  are calculated and compared between CO-DAC and CO-DACT methods. The flame is located around the location  $X = 1.25$  cm. It is seen that the CO-DACT method is accurate and agrees very well with the CO-DAC method for all the regions including burned region, unburned region and flame surface. Compared with the flame surface location (i.e., the flame speed), the relative error in space is only 0.3%. The excellent agreement demonstrates that the CO-DACT method is good enough to capture the major flame properties, including temperature and major species distributions and the flame speed.

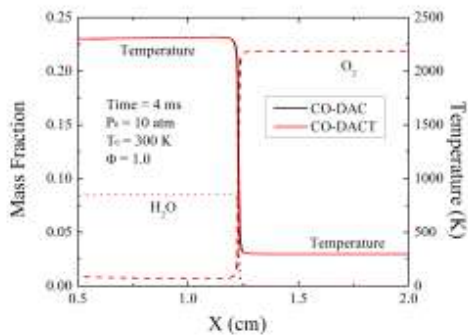


Fig. 3 Distributions of temperature and major species ( $O_2$  and  $H_2O$ ) at 4 ms.

Figure 4 plots the total CPU time comparison of the three different methods for a spherical flame propagation. The red, blue and yellow sections represent the CPU time used for

transport properties, diffusion flux, and convection flux, respectively. The black section is the CPU time for solving the chemistry. This figure clearly shows that compared with the original HMTS method for chemistry integration, the HMTS/CO-DAC model can accelerate the reaction calculation by a factor of 2 via on the fly model reduction. However, the time required for transport properties remains unchanged and is the most time consuming process. The present HMTS/CO-DACT method can dramatically reduce the CPU time for transport properties and increases the overall computation efficiency compared with the original HMTS methods.

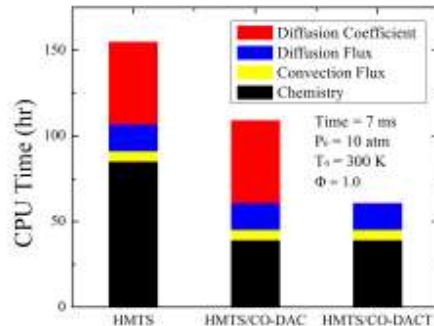


Fig. 4 Total CPU time comparisons between different methods for chemistry, convective flux, diffusion flux, and transport properties at 7 ms of spherical flame propagation.

### III. CONCLUSION

The A computationally efficient, correlated dynamic adaptive chemistry and transport (CO-DACT) method is developed for combustion simulations using a large detailed chemistry and transport model. The results showed that the CO-DACT method is accurate and computationally efficient. In flame calculations, the present CO-DACT method is about more than 200 times faster than the original mixture-averaged diffusion model for computing the transport properties. The relative error in flame speed is linearly dependent on the threshold value for constructing the phase space.

### ACKNOWLEDGMENT

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