# LARGE EDDY SIMULATION OF REACTIVE FLOW ON THE FIRE SIDE OF A STEAM CRACKING FURNACE

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There has been a tremendous increase in the production of ethylene over the past couple of decades and this trend is expected to continue in the foreseeable future as well. Steam cracking- the principal process used for the production of ethylene has gained increasing interest, both at a fundamental as well as at a systems level, with the ultimate objective of making ethylene production energy-efficient and lesser polluting (*https://improof.cerfacs.fr/*).

Numerical studies published in the past used Reynolds Averaged Navier-Stokes (RANS) equations coupled with the Radiative Transfer Equation (RTE) to solve for the mean flow field. However, for gaining deeper insights about the combustion occurring inside the furnace, unsteady flow features need to be captured using accurate and proven numerical techniques such as Large Eddy Simulation (LES). The challenges associated with LES of steam cracking furnaces include the presence of large spatial and temporal scale separation and the concomitant high computational cost, modeling accurate and sufficiently detailed chemistry to predict combustion and incorporating radiative heat transfer effects. In this study, the LES of a steam cracking furnace is carried out for the first time, by addressing the first two of the above-mentioned challenges using novel numerical methods and chemistry reduction techniques.

Although LES solvers based on explicit time integration schemes, such as AVBP (www.cerfacs.fr/avbp7x), exhibit excellent numerical resolution and accuracy, they are limited in the maximum allowable time step that can be used, due to numerical stability requirements. This limitation is aggravated even further in the case of simulations of furnaces due to small time steps and large flow-through times. In this study, this issue of stiffness is addressed using a novel acceleration technique based on local time-stepping coupled with overset grid methodology. The acceleration technique is validated on multiple test cases and shown to incur a minimum loss in simulation accuracy. The technique is used in the current simulation and speedup by a factor of 4 was observed.

Accurate prediction of temperature, heat release and pollutants inside the furnace requires accurate chemistry at a reasonable computational cost. In this study, a recent and detailed chemical mechanism for methane combustion is analytically reduced using the classical DRGEP method and QSS approximation tool ARCANE (*https://chemistry.cerfacs.fr/en/arcane/*). The reduced mechanism is validated with the detailed one and found to reproduce all the relevant chemical features of the detailed scheme accurately.

In this paper, the LES simulation results are compared with available measurements of temperature. This study emphasizes the need for the engineering community to embrace LES as a furnace and burner design tool by demonstrating its application on a real steam cracking furnace.

## Introduction

Light olefins such as ethene, propene and 1,3- butadiene are essential inputs to the petrochemical industry. The myriad products from these industries have become an indispensable part of our lives today. The demand and production of such olefins have been increasing over the decades and are assessed to be so in the future as well. Steam cracking is the principal process by which olefins are produced from alkanes today and is a major consumer of primary energy- consuming close to 8% of the total industrial energy consumption. The petrochemical industry also contributes to greenhouse gas emissions and hence to global warming- 21% of the total global emissions is estimated to be from the industrial sector, out of which 23% is contributed by the petrochemical industry alone [1]. Hence, any attempt to improve the energy efficiency of steam cracking furnaces is desirable from an economic and environmental stand point.

Numerical simulations are increasingly replacing experimental tests to design combustion systems due to their marked cost advantage and due to the huge amount of data obtained from numerical simulations which can hitherto be obtained from tests. In the past, many numerical simulations of cracking furnaces have been carried out by researchers in the petrochemical industry. Two of the early researchers to carry out such studies were Lobo and Evans [2]. They studied the heat transfer occurring inside furnaces using empirical models for different fuels. Rigorous numerical studies focusing on the reactor side of the furnace began since the 1970s. Robertson and Hanesian [3] modeled the reactors inside the furnace as ideal plug flow reactors (PFR) using a 10 species 6 reactions mechanism. Similar studies were performed by researchers [4]-[7] with emphasis on the reactor side while the furnace was modeled using zonal methods and the convective heat transfer on the reactor coils modeled using known correlations. Detemmerman and Froment [8] carried out one of the first coupled simulations of the furnace and reactor coils using a Reynolds Averaged Navier Stokes (RANS) solver and a 3-step 6-species methane-hydrogen chemical mechanism. Other researchers [9]-[11] followed suit and used k-ɛ RANS solvers along with the EBU combustion model to analyze methane-hydrogen combustion. Tang et al. [12] used a transported probability density function (PDF) model with in-situ adaptive tabulation for studying lean premixed combustion in low NOx burners while Han [13] and Lan [14] studied a coupled furnace reactor system using the presumed PDF approach. In recent years, researchers [15]–[18] have used k-ε RANS model with simple eddy dissipation combustion models coupled with discrete ordinate method (DOM) for simulating radiative heat transfer.

While LES has matured to a level of being used as a design tool in the aerospace and automobile industry today, the perpetual dependence on RANS in cracking studies is primarily due to the challenges associated with running LES in a computationally feasible manner. This is due to the presence of a large spectrum of spatial (from less than a millimeter (mm) near the fuel nozzles to more than 10m height of the furnace) and temporal (from 10<sup>-8</sup> seconds near fuel injection to a flow-through time of 5 seconds) scales. Requirements on the grid spacing and time steps to adequately resolve most of the relevant flow and chemical scales and the numerical conditions associated with stability such as that on the CFL number, largely restrict the speed of computations. One way to circumvent this is to use implicit time integration schemes that allow (from a stability standpoint) much larger time steps. However, implicit schemes suffer from poor dispersion relation preservation properties as explained in [19]. Also, the actual computational benefit obtained using implicit schemes is often debated due to the high cost of matrix inversions. An alternative way to speed up computations is to use local time stepping based explicit time integration schemes and are broadly classified as hierarchical and non-hierarchical methods. Hierarchical methods comprise of adaptive mesh refinement methods such as [20]-[22]. Non-hierarchical schemes are based on asynchronous local time-stepping [23], [24] or domain decomposition based local time stepping such as [25] and are based on non-adaptive, unstructured meshes suitable for simulating complex geometries.

The need for incorporating sufficiently detailed chemical mechanisms in LES cannot be understated if the

thermochemical properties of the system need to be simulated accurately. Most of the earlier works in the field of furnace simulations used simplified chemistry involving 6-10 species and less than a dozen chemical reactions to keep the computational costs low. Detailed chemistry effects are incorporated in methods that can be broadly classified as flamelet like or PDF based [26]. While flamelet based methods invoke flamelet assumptions and rely on reducing the complex chemistry to a lower dimensional manifold, PDF based methods are costly to be used in such studies. With the computational power increasing over the years, one can now think of solving species transport equations obtained after reducing a detailed chemical mechanism. Many such reduction techniques exist, out of which analytical reduction methods (ARC) is gaining popularity. The full chemical mechanism is downsized using the quasi-steady state assumption (QSSA) and directed relation graph methods to a computationally tractable (20-30) number of species.

In the present study, LES of a steam cracking furnace is carried out. Methane at ambient conditions is used as the fuel. A novel method using local time-stepping similar to the work of [25] is used to accelerate the computation. A recent, detailed mechanism for C1-C3 hydro-carbons is analytically reduced. This mechanism is validated with the detailed mechanism for representative one-dimensional flames. The LES acceleration technique along with the reduced mechanism is used to study reactive flow inside a steam cracking furnace for the first time in published literature.

This paper is organized as follows. Firstly, the experimental test furnace facility is described followed by a description of the computational domain. The LES acceleration technique, LESAULTS, is elucidated along with its validation on a vortex convection test case. The analytical mechanism reduction is then detailed. Finally, the results of LES of test furnace is discussed.

### **Experimental Configuration:**

The test furnace chosen for the present study is located at the JZHC facility at Tulsa, Oklahama, USA. The furnace is used to test the performance of steam cracking burners. A schematic of the furnace is shown in Figure 1(a). The furnace has dimensions of 14m x 2m x 3m. 8 reactor coils are positioned vertically facing the burner. Water at controlled flow rates and known temperature is pumped through the coils to mimic the process gas flow. 4 of the coils located closest to the two burners are thermally insulated completely using composite fiber. Two coils one either side of the furnace center line are thermally insulated only on the fire side while the remaining two are left uninsulated. The furnace houses two COOLstar® Ultra low NOx burners. Ambient air enters horizontally through the muffler (not shown) into the burner plenum. The air is deflected vertically upwards by a baffle and leaves the burner vertically. The fuel entering the manifold is split into 9 different fuel risers located circumferentially around the burner. Five of the risers are connected to primary fuel nozzles which inject fuel both radially into the burner center as well as vertically upwards. The remaining number of risers are connected to staged fuel nozzles which eject the fuel only vertically upward. The fuel and air temperature are 298 K and 294 K respectively and the pressure of incoming air is 1 Atm.

## **Computational Setup:**

The test furnace configuration enjoys geometrical symmetry with respect to a vertical plane passing in between the two burners. Taking advantage of this, only one half the configuration comprising of a single burner and 4 reactor coils is simulated in this study. A schematic of the full computational domain is shown in Figure 1 (b) along with the nomenclature of the relevant planes and the various boundary conditions used. The air and fuel inlets are simulated using characteristic based inlet boundary conditions with specified mass flow rate, temperature and gas composition. The outlet is also simulated as characteristic based

outflow boundary condition with a relaxation coefficient specified to fix the target pressure. All the walls are simulated as adiabatic. The cooling flow through the reactor coils act as heat sinks in the furnace. Hence, they are not geometrically modeled; instead, a uniform heat loss is applied on the projected area of the coils on the furnace wall. The fuel is treated as pure methane and all the gaseous species are treated as perfect gases.



Figure 1. (a) A schematic of the test furnace and burner simulated in the current study. Mixture fraction field on the horizontal plane passing through fuel nozzles is depicted in inset to show fuel injection pattern and fuel-air mixing (b) The computational domain and boundary conditions used.

### LESAULTS Method:

In this method, portions of the computational domain which require low time steps are identified and the computational domain is split into multiple, overlapping subdomains each run with its maximum permissible time step. The time step used in each sub-domain is chosen as an integral multiple of the smallest time step among all sub-domains. for easy synchronization. The governing flow equations are solved in each of the sub-domains independently of the other using this local time step. When time integration in all subdomains reaches a common flow time, flow information is exchanged between the sub-domains at the overlapped regions. An asymmetric stencil is used for the information exchange since the error (arising

from non-accurate boundary conditions) from the domain boundaries propagate in an asymmetric manner. The computational speed up is obtained by proper load balancing of computing cores dedicated to each of the sub-domains. The computational speedup, S, for a collection of N such overlapping sub-domains and a negligible number of nodes in the overlapped region is given by,

$$S = \frac{\sum_{j=1}^{N} \frac{P_j}{\Delta t_{min}}}{\sum_{j=1}^{N} \frac{P_j}{\Delta t_j}}$$

Eqn. 1

Where  $P_j$  and  $\Delta t_j$  refers to the number of nodes and the time steps used in the j<sup>th</sup> sub-domain respectively.  $\Delta t_{min}$  is the minimum of time steps among all the sub-domains.

A schematic of the LESAULTS methodology applied to two sub-domains is shown in Figure 2(a). Here Sub-Domain<sub>small</sub> contains N<sub>small</sub> number of small cells of size  $\Delta x_{small}$  which impose a small time step ( $\Delta t_{small}$ ) and Sub-Domain<sub>large</sub> comprises of N<sub>large</sub> cells which allow a larger time step ( $\Delta t_{large}$ ). Sub-Domain<sub>overlap</sub> is shared by both the sub-domains and permit time step ( $\Delta t_{large}$ ) used in Sub-Domain<sub>large</sub>. The theoretical speed up S for such a configuration as a function of the ratio of the number of cells R<sub>n</sub> = N<sub>large</sub>/N<sub>small</sub> and the ratio of the time steps R<sub>ot</sub> = ( $\Delta t_{large} / \Delta t_{small}$ ) is shown in Figure 2(b). It can be observed that S asymptotically reaches the value of R<sub>ot</sub> as R<sub>n</sub> tends to infinity. Hence, LESAULTS technique performs best for

configurations in which a few small cells dictate the time step in the overall computational domain. The present study is an apt candidate for LESAULTS method to be used, since the smallest time step is dictated by the small number of extremely fine sized cells located inside the fuel nozzles.







(b)

Figure 2. (a) A schematic of the domain decomposition used in LESAULTS method applied to two sub-domains. (b) Computational speed up as a function of time-step ratio  $R_{\delta t}$  and cell number ratio  $R_n$ .

#### computational speedup obtained.

#### Analytical Chemistry Reduction:

## Validation:

The LESAULTS method is validated on multiple test cases out of which an isentropic vortex convection is described below.

#### 2D isentropic vortex convection:

The convection of an isentropic vortex in an inviscid flow with periodic boundary conditions on all the four sides of the rectangular computational domain is a typical test case to study the dissipation and dispersion characteristics of numerical codes. The LESAULTS method is validated using this test case. The computational domain (rectangle in shape) is divided into three sub-domains (D1, D2 and D3) with overlapping regions between D1 and the other two domains as shown in Figure 3. Time step of 1.0x10<sup>-7</sup> sec and 1.0x10<sup>-6</sup> sec are used in D1 and the other two domains respectively (corresponding to  $R_{\delta t}$  =10). Grid cells of sizes 1.55 mm and 15.5 mm are used in D1 and the other two domains respectively. Inviscid flow simulation is carried out and the non-dimensional pressure obtained using LESAULTS and the conventional solver is shown in Figure 3 at three different time instants after the vortex convects through domain interfaces. It can be observed that the vortex convection is simulated as accurately as the conventional simulation in addition to the

In this study, a reduced mechanism is derived from a recent, detailed mechanism (hereafter referred to as POLIMI mechanism) for C1-C3 hydrocarbons [27] which has been validated for its NO sub mechanism. The detailed mechanism consists of 151 species and 2357 reactions and the reduction is carried out using the chemical mechanism reduction tool ARCANE<sup>1</sup>. The analytical reduction is carried out in three steps: Species and reaction reduction using Directed Relational Graph with Error Propagation (DRGEP), species reduction using species lumping and finally using the QSS assumption. In the present study, the reduction is carried out using 1D unstretched premixed flame at ambient temperature and pressure conditions and 4 different equivalence ratios as the target flame. The maximum relative error allowed on flame speed is set to 5% and

<sup>&</sup>lt;sup>1</sup> Website: <u>https://chemistry.cerfacs.fr/en/arcane/</u>

The reduced mechanism is now

that on CO and CO2 production rates is set to 10% of that predicted by the full mechanism. A reduced mechanism consisting of 25 transported species, 19 QSS species and 398 reactions is obtained after full reduction.



verified with the detailed mechanism for one dimensional flames. 1D premixed, methaneair flame at ambient conditions is simulated for a range of equivalence ratios using the tool CANTERA<sup>2</sup> for the detailed as the reduced well as mechanisms. The results obtained are shown in Figures 3 (a) and (b). The laminar flame speed obtained using the reduced mechanism is found to be within 3% deviation from the detailed mechanism while the maximum temperature showed a deviation of less than 5 Kelvins. The total CO and CO2 production rates in the flame are

Figure 3. Comparison of the non-dimensional pressure profile predicted by conventional LES and LESAULTS

shown in Figure 3(b) and is found to be within 10% deviation from the detailed mechanism.



Figure 4. 1D premixed flames: Comparison between reduced and detailed mechanisms. (a) Flame speed and Max. Temperature. Error bars correspond to +/- 3% for laminar flame speed and +/- 5K for temperature (b) CO and CO2 production rates. Error bars are +/- 5% of detailed mechanism.

<sup>&</sup>lt;sup>2</sup> Website: <u>https://cantera.org/</u>

### **Results**

The LESAULTS method along with the reduced mechanism is used in the LES of the test furnace. In order to apply LESAULTS, the computational domain is divided into three sub-domains (AVBP01, AVBP02 and AVBP03) and is shown in Figure 5 along with the time steps and representative mesh element sizes used in each of these sub-domains. AVBP01 contains the fuel injection holes and hence very fine elements and an extremely small time step of 1.0x10<sup>-8</sup> s is used here. Since the flame is anticipated to be located in AVBP02 relatively fine elements and a larger time step (1.0x10<sup>-7</sup> s) is used here. AVBP03 shall comprise mostly of the plume and a much coarser mesh and a larger time step (1.0x10<sup>-6</sup> s) is used.

LESAULTS method with the above-mentioned domain decomposition strategy is used to carry out LES. Sigma model was used for the sub-grid scale closure. The simulation was carried out for an overall flow time of 20 secs (corresponding to 4 flow-through times in the furnace). A total of 720 computing cores were used to simulate all the three sub-domains. Calculation with the LESAULTS method was found to be 3.4 times faster than the conventional LES. This value of speed up is close to its theoretical estimate of 3.6 obtained from Eqn. 1. It is to be emphasized that this value of speed up can be further improved by optimizing the domain decomposition strategy and mesh element distribution. With an a priori albeit preliminary knowledge of the flow in the system, regions demanding small time steps can be identified and element sizes judiciously chosen to speed up the computations even by an order of magnitude. Since the computational cost to perform a conventional LES (without LESAULTS methodology) is exorbitantly high, a comparison of the current results with a conventional LES methodology is not presented in this article. The results of the LES simulation with LESAULTS method is elucidated in the following paragraphs. Since temperature inside the furnace is the only data measured experimentally, the same is compared with the corresponding calculated values.



Figure 5: Domain decomposition strategy used in the simulation of test furnace

Figure 6: (a) Schematic of a vertical plane passing through burner center along with nomenclature of various locations. (b) Time averaged vertical velocity component on the mid-plane of the burner

Flow Field Time-averaged vertical velocity component on a vertical plane passing through the burner center is visualized in Figure 6 (b). along with the location and nomenclature of various planes discussed in this section shown 6(a). After combustion Figure occurs near the burner, the hot combustion products rise upward and gradually lose heat near the front furnace wall where the reactor coil heat loss is applied. This results the formation of a strong in recirculation zone, (RZ<sub>1</sub>). A portion of the recirculating flow from RZ<sub>1</sub>, skims along the furnace walls and the symmetry plane and eventually gets entrained by the burner jet near the rear furnace wall. This results in the high values of the vertical velocity component observed near

the rear furnace and burner walls. The entrainment of  $RZ_1$  slightly bends the burner jet flow direction causing an additional, weak recirculation zone ( $RZ_2$ ) close to the rear furnace wall.  $RZ_1$  has a height of 4m while  $RZ_2$ 

is relatively weak in strength and measures only 1.5m in height. Farther downstream of RZ<sub>1</sub> and RZ<sub>2</sub>, the velocity is reduced although its profile on a horizontal plane peaks closer to the front furnace wall.

## Flame Shape and Thermal Field

A stable flame with two distinct combustion zones is found to occur inside the furnace. Figure 7 depicts these combustion zones inside the burner. Primary fuel nozzles eject fuel radially inwards into the burner. These jets react with fresh incoming air from the burner plenum to form the primary flame zone. This primary zone is compact in size (occupying 0.25% of furnace volume) and is located completely inside the burner. On the other hand, the vertical fuel jets skim along the outer walls of the burner, mixing with the recirculating flue gas, eventually burning and stabilizing on top of the burner tile as shown in Figure 7. This forms the secondary flame zone and is much larger in size.



Figure 7: Schematic of the cross section of the burner passing through a primary fuel nozzle

This can be observed from the time-averaged temperature field at a horizontal plane immediately downstream of the burner tile shown in Figure 8 (a). The high temperature zones on the tile walls indicate secondary flame anchoring. High temperature region can also be observed near the burner rear wall due to the entrainment effect of RZ1 as explained previously.

An iso-surface of mean temperature in the secondary combustion zone in the furnace is shown in Figure 8 (b). The flame is approximately 3m in height and is found to occupy 25% of the total furnace volume. 92% of the heat of combustion is found to be generated in this zone which aids in heating the process gas.

A comparison of the measured and calculated temperature inside the furnace is shown in Figure 9. An overall good

agreement is seen between the values. Temperature is over predicted in the mid-furnace. This is anticipated as radiative heat transfer has not been taken into account in this study.



Figure 8. (a) Mean temperature field on a horizontal plane downstream of burner tile. (b) Iso-surface of temperature at a value of 1600 K. Mid-plane is coloured by mean temperature field



Figure 9: Comparison of calculated and measured temperature at three different locations in the furnace. Furnace floor, Furnace middle and Furnace top are located at heights of 0.15m, 5.6m and 10.9m from the furnace floor respectively

Figure 10 shows the linear variation of timeaveraged mass fractions of CO2, CO and NO on horizontal planes located at 1,2, 5 and 10 diameters downstream of the furnace floor. The burner center axis is located at x = 0.

The CO2 mass fraction exhibits a nearly flat profile for planes with y/d=5 and 10 with their values close to that of equilibrium values. This is indicative of complete combustion and high residence time of the recirculation zones. For y/d=1 and 2, low non-zero values of CO2 mass fraction is observed on the burner centerline due to the combustion occurring in the primary flame zone.

The high temperature region near the rear furnace wall is conducive for the oxidation of methane to form CO. This can be observed from

the regions of high CO mass fraction near the rear furnace wall observed till y/d = 5. Downstream of this plane, the CO mass fraction tends to decrease due to its oxidation to CO2. The location of peak CO mass fraction is also observed to shift to the right as one moves downstream, due to the bending of the flame due to recirculation zone. The high temperature zone near the rear furnace wall causes NO to be produced through the thermal mechanism as can be observed from the NO mass fraction values on all horizontal planes. The high temperature zone near the front furnace wall at y/d= 5 also explains the region of high NO at x = 0.8m. Downstream of this plane, the NO profiles tend to acquire a uniform profile.



Figure 10: Time averaged CO2, CO and NO mass fraction at horizontal planes 1,2,5 and 10 diameters above furnace floor

## Conclusion:

LES of a steam cracking furnace is carried out for the first time in published literature. Due to the numerical stiffness associated with multiple scales, a novel method (LESAULTS) for LES acceleration is designed. This method is validated on academic test cases is found to simulate results in excellent agreement with the conventional LES method. A new, reduced mechanism was derived from a recent detailed mechanism for methane combustion. The LESAULTS method was used in conjunction with the analytically reduced mechanism to study the reactive flow inside a test furnace. A comparison of measured and calculated temperature at three locations inside the furnace showed good agreement. Inclusion of radiative heat transfer into the LES simulation will be attempted by the authors in the future and is anticipated to show even better agreement to measurements.

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