EFFECT OF CLUSTERING ON REACTOR NETWORK MODELS

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Abstract
Predicting the formation of pollutants from combustion devices requires the combination of accurate CFD and detailed kinetic mechanisms. A possible approach to handle this problem consists in post-processing the related CFD results, obtained through a simplified kinetic scheme, with detailed mechanisms.
This is done by the *Kinetic Post Processor* (KPP), a tool developed at Politecnico di Milano, able to estimate the emissions of compounds like NO_x, CO and PAH with the required accuracy. Nevertheless, even by using a post-processing technique, this evaluation may be particularly heavy from a computational point of view, especially when dealing with realistic, full-scale models.
In these cases, the corresponding reactor network model can be unburdened by grouping (or *clustering*) cells, which are similar from a fluid dynamic and kinetic standpoint. Literature shows that although in this way the original fields of motion and temperature are altered, its impact on the output can be negligible and the results close to experimental measures.
The recent availability of a parallel version of the software has extended its potentials, thus making possible to work with reactor networks made up of $10^5 \div 10^6$ reactors and kinetic schemes of 50÷100 species. Therefore, it has been possible to test models of devices without any kind of cells' clustering.
In particular, in this paper a sensitivity analysis to clustering of a case study (a low-NO_x combustor) has been carried out and discussed; as a feedback, the output levels in terms of NO and CO are evaluated. The results provided important indications from two different point of views: the impact that clustering can have on pollutants when modeling complex devices, and the importance of the upstream CFD simulation when evaluating emissions through a post-processing strategy.

Introduction

The great importance held worldwide by combustion technologies (90% of the global produced energy) must deal with the strict limitations in terms of emissions of pollutants. As a consequence, the ability to design devices able to stay within these limits has become crucial for the industry world.

In this scenario, the role played by computational tools for predicting emissions has been constantly growing in the latest years, although the complexity of combustion phenomena places significant challenges from the modeling point of view (particularly when dealing with turbulent flows). Indeed, in order to ensure a sufficient degree of truthfulness to the concerned models, it is necessary to combine two different factors: an accurate fluid dynamic (CFD) model of the equipment and a detailed kinetic mechanism. From a computational point of view a direct coupling, which basically solves material, momentum and energy balances all together is unfeasible, even with the most modern, distributed memory machines. For this reason the development of approaches to obtain results in reasonable times is related to doing some assumptions about one of the mentioned aspects.
A possible way to keep accuracy on both CFD grid and kinetic scheme consists in splitting the resolution procedure into successive steps, as it is done in post-processing techniques. Basically, they evaluate the desired output in three stages:

1. First, they solve a detailed CFD model of the device through a simplified (skeletal) kinetic scheme, able to describe the behavior of the major species;
2. Then, an equivalent reactor network model is created and CFD outputs are imported into it, conserving the temperature and flow fields.
3. Finally, the isothermal reactor network is solved with a detailed kinetic mechanism and results are evaluated.

Literature shows [1, 2] that this methodology has been successfully tested on several cases, and results in terms of emissions of pollutant compounds are in good agreement with experimental data.
Nevertheless, for industrial size cases, the heaviness of the reactor network can still be excessive for obtaining results in acceptable times; for this reason, its number of elements may be decreased, compared to the CFD grid, by grouping (or *clustering*) cells which are similar from a fluid dynamic standpoint, such that the expected kinetic behavior can be assumed as the same. In particular, in this paper this strategy is analyzed in detail; its performances are tested in the case of *Kinetic Post Processor* (KPP), a dedicated tool developed at Politecnico di Milano.

KPP: model and resolution

Following the post processing approach previously described, the Kinetic Post Processor is based on one fundamental, verisimilar hypothesis: minor species, like radicals and pollutants, do not affect temperature and motion fields because of their minimal presence. Therefore, those fields can be evaluated with a simplified scheme, entered into one of the available CFD codes (e.g. FLUENT or OpenFOAM®). Then, a network of perfectly stirred reactors is created, whose fluid dynamic conditions are imported from the previous stage and kept fixed. The composition obtained for the major species are used as a first guess for the final step (Figure 1):

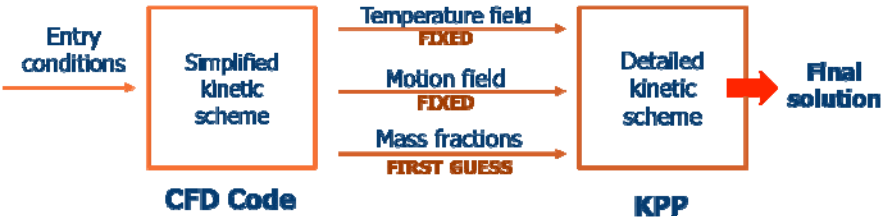

Figure 1. KPP resolution logic

The fact of fixing temperature and motion fields allows to decouple material balances, and energy and momentum ones: thus, only the former need to be solved, and the number of equations to be solved decreases, but especially their non-linearity. The resulting system is made up of $NC \times NS$ equations, where NC and NS are respectively the number of cells and species. For the j-th reactor and the i-th species, they have the following form:

$$\dot{m}_{tot,j}\left(\omega_{j,i}^{in} - \omega_{j,i}^{out}\right) + \sum_{k=1}^{N_{AD}}\left(\vec{J}_{j,i,k} \cdot S_{j,k}\right) + V_j \cdot MW_i \cdot \sum_{p=1}^{N_R}\left(\nu_{i,p} \cdot r_{j,p}\right) = 0 \qquad (1)$$

where ω are the molar fractions, J the (turbulent) diffusion flows, S the interface surfaces and r_p the reaction rates.

Overall, a non-linear system must be solved, whose Jacobian for a structured grid is made up of blocks, which are dense on the main diagonal and diagonal outside (Figure 2):

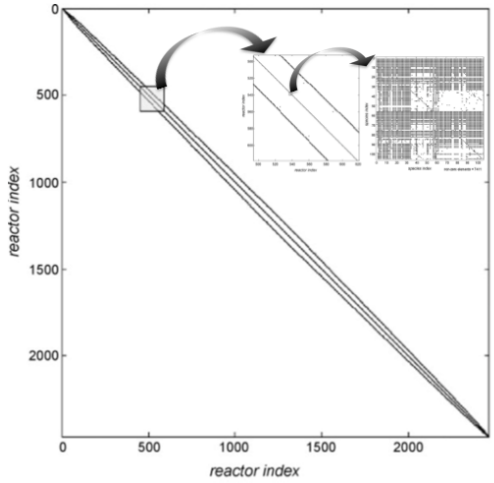

Figure 2. Boolean structure of the Jacobian matrix of the system (adapted from [3])

Newton's method is not robust enough to directly find the solution; therefore, the system is solved through an iterative strategy, which progressively approaches the solution, applying Newton's method only when residuals are low enough.

Cells clustering

CFD models of industrial cases may be even made up of $10^5 \div 10^6$ cells; if a kinetic scheme of 100 species is used for post processing, overall a non-linear system of up to 10^8 equation may result, with a huge consumption of memory and computing power. Without the adoption of parallel systems, it has been seen that the available tool is not able to solve systems larger than $\sim 3 \cdot 10^6$ equations for memory reasons (on a system with 36 GB RAM). Alternatively, the number of reactors may be reduced by adopting a smart operation of cells' clustering: in the less critical regions, e.g. where temperature is low and/or temperature gradient is not too high, adjacent cells can be grouped; on the other hand, the level of detail is kept higher in higher-temperature zones, where kinetics are faster (and reaction rates increase in a non-linear way). Therefore, according to the degree of clustering required, it is possible to regulate the number of cells, and consequently the size of the problem. Of course, if the number of cells is excessively reduced, the initial CFD grid is completely altered and so will be the output of the program in terms of emissions.

Effectiveness of cells clustering

The effectiveness of this approach to clustering strongly depends on the level of approximation of CFD field introduced by merging more cells. Previous experience about KPP [1, 3] shows that, by investigating turbulent, lab scale jet flames, the number of cells could be reduced up to one tenth, without losing in accuracy for NO and CO emissions. Nevertheless, a general rule cannot be deduced: it strongly depends on the specific fluid dynamics. As a matter of fact, when dealing with industrial devices, their CFD models are much more complex, and the alteration brought about by even a low degree of clustering may be significant. In the following, a case study which shows the effects of cells' grouping in a complex grid is reported.

The case analyzed is an axially staged, low-NO_x combustor for aero-engine turbofan, built up and studied experimentally by AVIO S.p.A. It had already been discussed by Frassoldati et al. [4], but the recent availability of a parallel version of KPP has allowed to analyze it with more detail. Indeed, differently from the mentioned work, it has been possible to post-process the network as a whole, i.e. without any level of clustering by using the recently available parallel version of KPP. Then, a sensitivity analysis to clustering itself has been performed. The CFD original grid is made up of 290,764 cells, and has been solved with a detailed kinetic scheme made up of 86 species and 1,427 reactions developed at Politecnico di Milano.

The results are shown in the following charts, in terms of NO/CO overall in function of the clustering level (Figure 3).

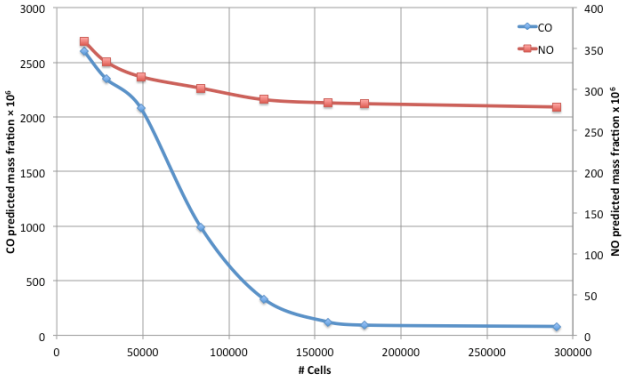

Figure 3. CO and NO sensitivity to clustering

In this case, below a number of ~170,000 cells, CO emissions are overestimated (up to a factor 30), while a better trend is observed about NO (whose error does not exceed 30%). The higher error in CO evaluation is to be attributed to its formation processes, which are fast if compared to the time scale of transport phenomena; its generation is then governed by fluid dynamics, which is altered due to clustering. Instead, the formation of NO is slower and then governed by kinetics: the alteration of fluid dynamics does not influence it at such a high extent.
These trends can be viewed in function of the radial coordinate (Figure 4 and Figure 5):

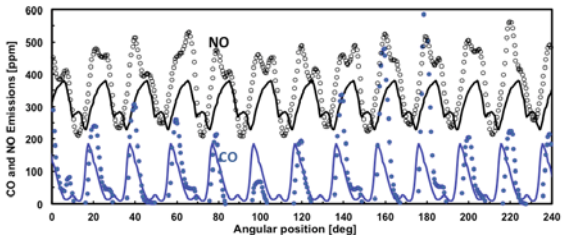

Figure 4. Predicted emissions without clustering vs experimental measures

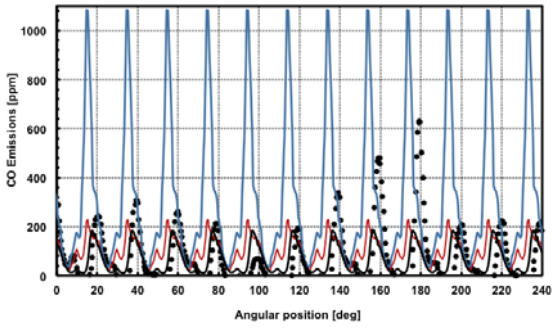

Figure 5. CO experimental data vs predicted. Black line = 290,764 cells (no clustering); red line = ~158,000 cells; blue line = ~120,000 cells

Without clustering, the predicted data about CO are in very good agreement with experimental data, while some discrepancies still remain for NO, especially for what concerns the emission peaks. Slight differences were also present between CFD fields and experimental data, as shown in [4]; this may have influenced KPP output, since a good CFD prediction is essential for the proper working of the tool.

Conclusions and future works

Among the available strategies to model turbulent combustion equipment, post-processing techniques allow to make the problem computationally affordable, although this might require the resolution of systems of even 10^8 equations.
In this paper, the opportunity of adopting a clustering strategy has been discussed; starting from the positive benchmarks already available in literature, an industrial case has been analyzed. Unlike the former, some limitations emerged, related to the impossibility to know *a priori* the minimum level of clustering, which allows not to lose in accuracy. Below this level, the output values can be completely wrong, in particular for those species whose formation is highly dependent on CFD fields. Therefore in these cases the current clustering strategy still needs to be improved.

Acknowledgments

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