SPECTRAL-LIKE APPROACH TO MODELLING THE LIQUID FUEL ATOMISATION PROCESS IN A REACTOR

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Abstract: The aim of the following work is to individualise and to deepen some numerical methods finalized to represent the spraying process of a liquid fuel in a combustion chamber. First objective is to reach an optimisation of the representation the mixing process which happens between fuel droplets and oxidiser gas to obtain a better combustion reaction. Since a functional representation of diffusion and convective terms in turbulent regime needs high order derivative, it's demonstrated that a spectral-like approach with *Compact Schemes* is able to simulate the atomisation mechanism. In this context, we have evaluated the opportunity to be able to reformulate the procedure of EPD's reconstruction by another very efficient functional expression to integrate *NS*.

Key-Words: Mechanical Spraying, Tribology, Numerical Stability, Turbulent Combustion

1. Introduction

In the last period, many studies are affording the problem of the optimisation about the combustion plants. In the peculiar case of liquid fuel combustion, the spray modelling, in the hypothesis of reducing the environmental impact, is a central issue. Then choosing to adopt a CFD (Computational Fluid Dynamics) approach to model the spray injection oriented to make in evidence some peculiar advantage in the context of the planning these kind of system are taking more and more place. The attention of this work is focused on the choice of a FV (Finite Volume) analysis respect a DNS (Direct Numerical Simulation) one. It's well known that the spectral methods are very important in the wide context of the numerical simulation. Here we adopt a spatial and temporal cutting off higher numerical order which have a computational low cost, meaningful stencil points decreasing. The approach chosen is compact schemes like Lele [5] and comes from an integral formulation of the quantities. After we have gone on supporting analogous processes that share Lele schemes reconstruction philosophy, (polynomial reconstruction by approximated data), and improving further the quality of schemes expressed in explicit way. The umpteenth step has been to design on implicit methods (polynomial reconstruction by staggering) that allowed us to arrive, by a fourth degree polynomial expression, to go beyond the results obtained compact schemes of fourth order, nearly, equalling the eightieth order, also by using a lower number of stencil points.

2. Problem's phenomenological representation

A combustion analysis of thermo-fluid dynamics phenomena must use adequate tools to represent the operative characteristics of the same process. As turbulent motion fields main characteristic is their irregular evolution in time and also extensive quantities (mass, motion's quantity, enthalpy) with high diffusion level it's joined to this, then a strong three dimensionality comes on smaller spatial scales than those joined to motion's whole. It's well known more that motion's turbulent fields are strongly dissipative, that is: a portion of kinetic energy, associated to untidy motion, is transformed into inner energy and so comes back at tidy motion expense. For this high diffusivity influences straight a reagent mixing than all phenomenological characteristic we have seen until now. In fact, just this property favours molecular contact and mixing between different chemical kinds both in presence and in and in absence of chemical reaction [8]. From this, since supporting field dynamic quantities are strongly conditioned by turbulent motion, their representation by direct simulation or by Large Eddy Simulation (LES) needs high powerful resolution's ability and calculus tools. Surely new technologies have developed themselves to increasingly advanced hardware resources but to make a correct phenomenological description of processes taken into account they don't need always ability so extreme. Actually, following on recent developments in computing sciences, new and wider research scenario are open by means of possibility to make up equally new investigation strategies derived from changed management and calculus abilities of modern computers. Of course, we need adequate methods for physic interpretation of the case under examination, from which the choice of efficient integration appropriate schemes respect to turbulent models that are deputed to the object of study of phenomenological physical representation. Spectral analysis is among theories that have greatest success in turbulent fluid dynamic field. For its highest accuracy and its highest resolution, it seems to have just the requirements to satisfy enough good the refinements degree wanted by this kind of study, where micro scales definition plays a central rule.

3. Problem description

Among fluid dynamic situations that can come true inside the context of processes of combustion the case of liquid fuel occupies a relevant place. These kinds of process are very common. It is sufficient to think about normal petrol inside internal combustion engine or about diesel oil plants for energy production. In fact, in this case, it is easier to control and manage fuel, besides this case offers the not negligible merits, joined to easier transportability, to be easily stored and easily handled. To make feasible a process of combustion of a liquid fluid it is necessary before atomise fuel, that is to reduce it in so adequate small parts (called droplets) to combine it easier with air in mixing ratios determining more or less spontaneous ignition conditions. In practise, oriented air to fragmenting action set is realised to increase touching surface between fuel and oxidiser gas to optimise both the process of mass exchange and energetic exchange between the two phases. It is well known that pulverisation process of a liquid jet is very laborious and that is object of deep study, ([12] [14] [18] [19] and others), and since at the beginning fluid shows itself in compact form one has recourse to specific devices to atomise this jet. All this is done by passing liquid fuel that shows itself like a very thin film across the terminal part of an atomiser that provides for introducing the jet, usually in conic form, into firebox. Others dedicates to this matter working in experimental field describe various methods to obtain liquid film disintegration [9] [12]. Main ideas deduced, also by maturated widely tested experiences so far, come from traces listed here:

- To subject film extremity to pulsing contraction stresses that produce a marginal disintegration by surface tension. During contractions, long trickles are ejected out of edge. They make large drops;
- For piercing the film uniformly to form small circular areas that, then, will be progressively atomised by coalescence and by different accelerations in long trickles, we lead waves forming inside liquid film by surrounding atmospherics disturbances. This for making interaction between fluids that come out very speedy from nozzle, with some pre heated air that provides to break further the liquid in the immediate closeness.

On those basis one sees as far as point it's basic to make ready adequate tools for a correct phenomenological representation but one must care too a deeper study about physic case.

4. Fluid dynamics of swirled jets

It is well known that pulverisation is a phenomenology influenced strongly by disturbances. These disturbances are understood from viewpoint of: pressure, liquid jet due to turbulence and gaseous means peculiarities in which jet is injected. In liquid jets with assail flow prevailing (trickles with thin layer form) jet simple vibration is enough to cause the break up of it the distance from atomiser terminal part in which this happens depends by viscosity; if this gets higher then distance grows by pressure, by surface tension, and by outlet speed. Viscosity influences considerably, on a cinematic plane, the quantity of liquid fuel that is going to be atomised. Surface tension takes part both in the breaking process of liquid film and in trickles coming from this break. Actually if surface tension become higher then obtained droplets are larger. Besides, it is also possible to demonstrate pulverisation is made in depending on air interaction, and it gets better by air density growing up. Droplets speed in a moving air jet gets lower, due to air friction, until a minimum speed. Then, they are regarded as gradient joined form. Evaporating and burning phenomena interfere with phenomenon development. Most part of used techniques to make small droplets, with lower working pressure, base themselves on liquid film formation (5μ of wedge) by passing liquid fuel trough narrowest slots, wholes, or ring shaped space, by nozzles of special shape and construction or by feeding still fuel in the middle of a spinning round disk or cup. Evaporating little droplets, travelling by stationary motion along gaseous media, aren't in their whole of spherical form and liquid inside them is not stationary. Deformations, oscillations, and internal circulation inside droplets of a burning jet have scarce effects on disintegration, except in strong impact effects with gases current. The coalescence phenomenon is an important function of impact energy between two currents with different speeds. Drops closest to nozzle mix themselves with recycled gases and can undergo coalescence effects by crashes. Great concentration of drops contributes to this phenomenon in atomised jet also far from burner. Also pulses generated by combustion favourite droplets mixing. To evaluate correctly the behaviour of an atomiser usually we need to realise the following conditions:

- Dimension and operative conditions to obtain the wished liquid mass flow rate.
- To have a certain spatial configuration of resultant jet.
- To obtain a good droplets medium diameter impose some dissipation characteristic.

For swirl giver we understand a system able to give air coaxial jets with a tangential component of speed. By this way, we generate a strong ring shaped whirlwind at burner exit. Adequate mechanical tools to make rotation are injectors that have gained great importance by their flexibility. There are different kinds of turbulent nozzles, all of them based on creation of speed tangential component, by mechanical trickles or by use of auxiliary fluid. Interaction between swirl and jet is responsible of flame greatest stability that can be due to different factors as for example:

- Swirl condition makes faster the combustion at flame and lifts it by floating in local speeds; at the same the action of swirling flow makes large zones of premixing.
- Swirl works as warmth source because it pushes hot products of combustion to mix with partially premixed reagents. Then we have an increase of residence time during which fuel, air, and products can coexist: this represents an important stability factor. However, one can also to demonstrate how an excessive swirl becomes instability factor by excessive recall of cold air from outside.
- Swirl places integration points on upstream and downstream swirl side, working as flames join.

Exposed all above we care on some problem aspects about mild combustion. Focalising our own attention on the opportunity to achieve combustion conditions with high efficiency and low polluting emissions. Gained experience in this fundamental field relative to gaseous fuel leaded some results that are well cited in gaseous fuel scientific literature [30]. The behaviour of a spray made by liquid fuel droplets (gasoline) and then interaction characteristic with a warm burner flow (air). Work aim has been the determination of concentrations trend inside fuel by changing temperature at gas entrance. So far, we have limited us to sheer transport because combustion by liquid fuel is a very complex phenomenology; in fact, there are bi-phase flows interactions with evaporation and coalescence processes and a high number of chemical reactions. Burner geometry effects have not been studied deeply as this appears to us pleonastic in this phase and out of work target.

5. Analysis of stability conditions

Problem of combustible carriage of species is described by a simulation in discrete phase, made by gasoline droplets in a reference Lagrange system. This phase consists on scattered spherical particles in the continuous phase and they are moved by swirled jet. The trajectory of these discrete entities such as mass and heat transfer from a phase to the other one has been calculated by using a connection between the two phases. Turbulence model adopted in this simulation have indicated actual possibilities to simulate a large range of discrete phase problems. The result of all this work of pre-processing consists to note that, chosen an appropriate turbulence model to describe this kind of phenomenology, a fundamental aspect is to trace particles. This has been made in Lagrangian way; in these conditions one has investigate on the behaviour of that characteristic parameter that is diffusion for seeing possible mixing condition as one can demonstrate diffusion gradient is related to permanence time inside combustion zone of fuel particles because of a connection with turbulent viscosity μ_t subsists [12]. This work has underlined the system strong dependence from injection conditions above all (swirl and air speed). Next step will be oriented to obtain abilities to manage phenomena of evaporating and of particles coalescence until to simulate reactive flows.

6. Numerical model approach

Turbulent models pushed computational and fluid dynamic experts to research numerical methods well done to represent physic phenomena that usually are studied by these sciences. Most of physic phenomena relative to turbulence characterise themselves to be defined by the introduction of suitable scale factors that are at the same function of spatial temporal range to which the same phenomena are related. After this, spectral methods was developed, they performed the problem of turbulent flows representation at least in a part on simple geometry and easy surrounding conditions [2]. Part of difficulties joined to surrounding conditions was overtaken by alternative, but not too-much, introduction techniques as DNS that takes aim to solve equations associated to analytical model until physic limits that are defined by so-called Kolmogorov scales. As well known, these scales are useful to define characteristic quantity respect to which we estimate functional parameters of physic model that represents specific turbulent phenomenology. Finite Difference (FD) schemes are one among best aids for this scales representation thanks to fact it gives possibility to solve in quasi-spectral way and, more, it can be used on not uniform meshes in the strict sense of the word by the imposition of surrounding conditions without specific limitations. To preserve freedom conditions in the choice of definition degree of mesh quasi-spectral methods are preferred in turbulent phenomena analysis. These make a kind of procedure that does not impose limitations on examined flow characteristics, but exceeds difficulties imposed by simple spectral methods and more admits alternative numerical representations. Since most of these phenomena is defined as motion composition with high frequency, that is with high wave's numbers, and tends to be described by waves with small amplitude, then some has sought to develop methods to refine, at the same stencil, accuracy high degree. In order to guarantee a better approximation on spatial derivative so far we have been moved by attention to study how to make up systems that minimise errors associated to dispersion phase. This target has been pursued by introducing schemes that use weight suitable coefficients for the construction of numerical derivatives obtained by makings discrete of central kind. Some of these schemes realises a fourth order approximation on stencil that are composed by seven points with a better resolution than explicit equivalents of higher order. Instead, Lele concentrated his research to representations that optimise the state of art by taking advantage of previous studies never used results because of calculus limitations. This optimisation is made with a particular care to logic related to implicit schemes, defining a methodology of general character both on descriptive plane and on properly constructive plane; these aspects are summarised in the so-called compact schemes theory. These schemes present the certain advantage that in comparison with traditional finite difference's methods offer a better representation of smaller length scales, at the same approximation. By coupling the use of finite difference schemes with spectral methods, we obtain a valid support just for the representation of this scale range (spatial). As this kind of schemes founds its own base criteria on possibility to individuate reference parameters, as integration step. Thanks to which both by a game of opportune linear combination of function values at level n and by an opportune of weight of values assumed by derivatives in adjacent points one is able to take values set of derivative functions. Compact schemes pointed out very convincing results about their validity compared above all with so-called classic methods for making discrete both on approximation plane and on accuracy [1][4][5][6][7][15]. Innovative aspects of this procedure consists in introduction of an approach to so-called integral methods that represents already alone a further develop of difference approximation theory of EPD. An umpteenth step forward has been done by coupling compact planning with intrinsic logic of finite volume method. This methodology is among most consolidated in numerical simulation contest and we are oriented to do an analysis of spectral kind; use of interpolation refined techniques results to be central to solve differential problems imposed by equations as the last one. Theme of polynomial reconstruction in cells by which we tend to treat comports conformability problems, because of various occurring difficulties in border representation, above all across passages that are relative to analytical transformation. To arrive to a significant result we need to choose with wisdom both the kind of integration grid and interpolator polynomial's degree, as to them quality parameters of error are related, like:

- High accuracy.
- Low dissipation
- Low dispersion.

We start by considering a certain set of functions. These are at the same a subspace base, and, in our case, are given as development in polynomial series and have orthogonal property; this gives to reconstruction process of function, which is going to be integrated, the possibility operate a subdivision into its valence domain in m parts. In those parts, the function is calculated as mean integral of filtered quantity for each single element. The advantage of this representation consists in easy manipulation of component functions also if this will be prejudicial to convergence speed, as stability problems rise up because of possible high degree of the same polynomial [4]. Being just versatility the main characteristic of that development, compensator for low accuracy compared with other methods, it is possible, by coupling double effect to vary both the number of parts in which the domain is decomposed and that in which sub domain is subdivided; (h-p method). In fact, advantages of this method are immediately shown by thinking on talk about purposely-generated grids in each sub domain, with the aim both to simplify calculus operations and to obviate conformability pre-requisites. By this way any problem, caused by possibility to be in front of geometrical situations hard to be represented, can be exceeded by a procedure like that adopted in FV case [1]. In fact, the tool used for making discrete gives us a throwing down of numerical instability index, but calculated during long periods of observation. For this, we are proceeding so that an equations system is generated, in this only polynomials with a degree as high as the kind of considered approximation compare and that offer the base on which to make reconstruction at a fixed temporal step.

7. Integral polynomial reconstruction

The choice done is not casual, in fact, this imposition permits us to arrive to an easier reformulation of implicit relation coming out from compact schemes theory brought back here for conveniences:

$$f_i^I + \alpha_p (f_{i+1}^I + f_{i-1}^I) + \beta_p (f_{i+2}^I + f_{i-2}^I) =$$
$$c_{p1} \frac{f_{i+1} - f_{i-1}}{2h} + c_{p2} \frac{f_{i+2} - f_{i-2}}{4h} + c_{p3} \frac{f_{i+3} - f_{i-3}}{6h}$$

Since the reconstruction operation is made by adopting this point as centre of reconstruction in the hypothesis to be in presence of a functional quantity expressible in integral form, the operation of making discrete can be taken back to an expression of finite difference kind. In which values of cell-centred are as more representative as more adequate is the grid kind on which it is supported. Here compact reconstruction gives us a coupled representation of integral mean values and of calculated flows on border coinciding to extreme points of interval. The results of that operation are compared with exact solution; as we can see by diagrams, flow function that is remade by classic compacts is less accurate than that one remade by integrals. If we suppose a solution able to be expressed by a formulation according to Fourier representation [4] [5] [6] [8], it comes out from the operation of making discrete for each state quantity then it is possible to lead an analysis of spectral character about the efficiency of those schemes. In this sphere, we illustrate spectral analysis results in the following diagrams (Fig. 1)-(Fig. 2)-(Fig.3).

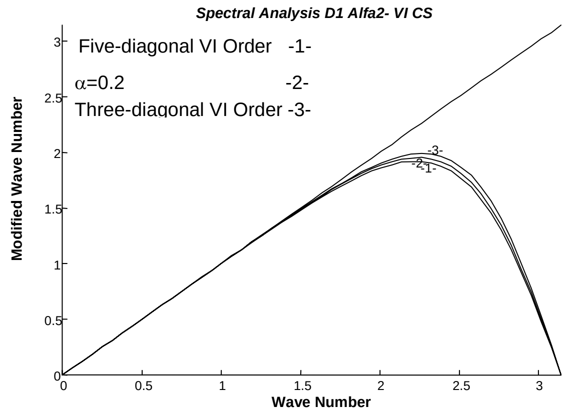

Fig. 1

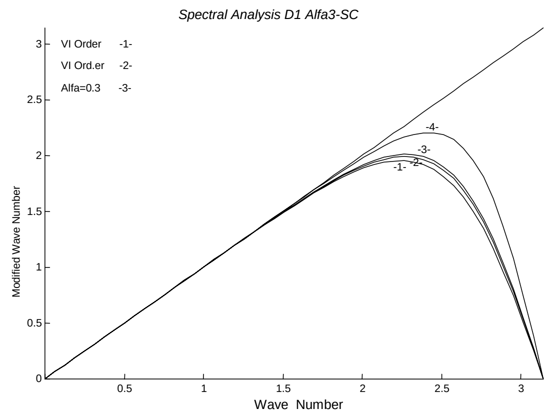

Fig. 2

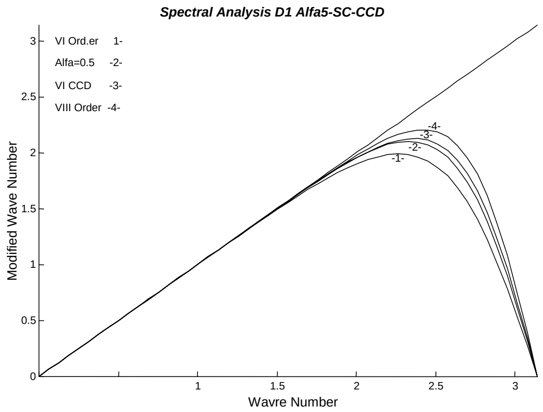

Fig. 3

A further improvement is obtained by reporting the double implicit condition on first derivative and the second one with α=0.5, as we are pointing after. (Fig. 4)-(Fig. 5).

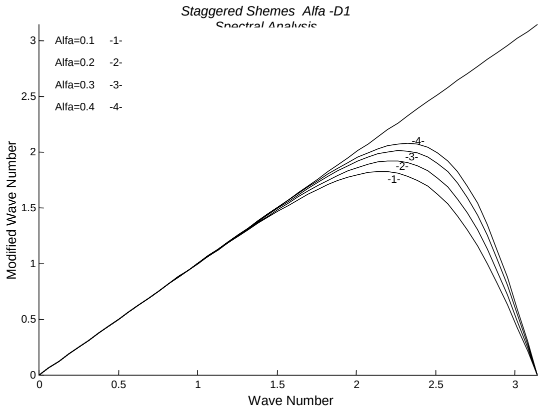

Fig. 4

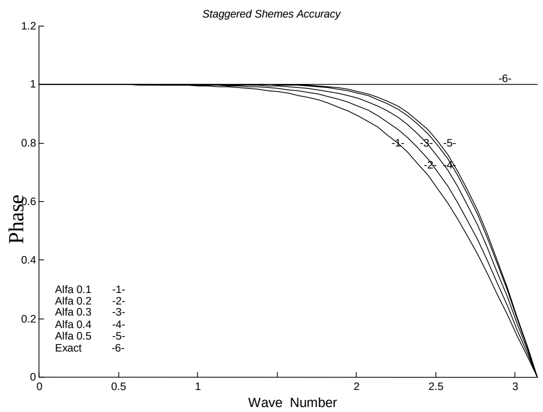

Fig. 5

Diagrams we have reported in the next give us a survey the validity and the efficacy of all we have said until now [20]; in fact, in the case of one-dimensional transports of passive scalars compared to simple analytical solution are tested in them (Fig. 6) - (Fig. 7).

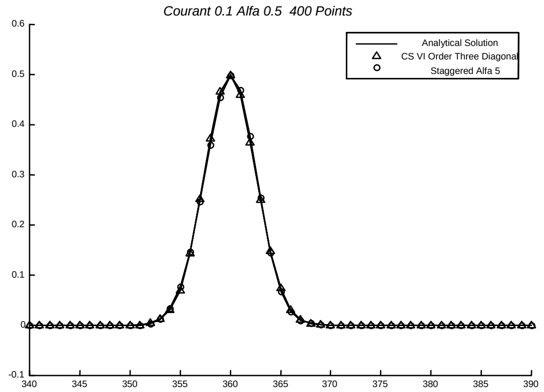

Fig. 6

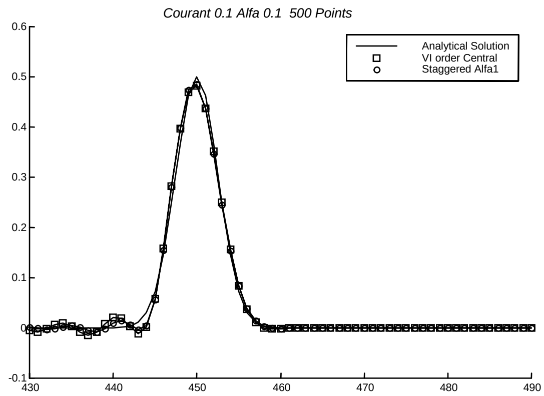

Fig. 7

8. Conclusions

As first realized target, the acquisition of required tools is showed to be able to determinate numerically a series of essential data for phenomenological description on case under examination. Among main parameters we individuate the dimension of fuel drops, their relative position and mixing state with air; to characterise them correctly we can't leave out of consideration about the proposition of admissibility requirement of an analytical-functional representation of Lagrangian-Eulerian kind for whole motion field. Since numerical models of greatest impact provide the use of a methodology for making discrete to cell-centred way, we start from this presupposition of approach to the problem exploring the possibility to avail ourselves of tools with high spectral efficiency. Then we open the horizon on a road oriented to extend to stronger integral formulations in reference to FV.

With this purpose we have effected an analysis about what are base elements of compact schemes theory to verify first the applicability and later the extensibility. A first objective has been achieved also if some difficulties have rise up before achieving our aim. In fact, some limitations imposed by re-constructive techniques on domains of two or three dimensions have appeared and have stopped the full completing of work prefixed plan. However, representation with lowest degree is a tangible proof of theoretic planning, also respect to results obtained by the simple Hermitian polynomial reconstruction with approximated data. Certainly we can't refuse this study is in testing phase and results here shown represent what one can call a first harvest of data. Scenes opened by this research already give a comfortable reading key of combustion phenomena in turbulent field.

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