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REVIEW PAPER

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NOVEL AREAS AND FUTURE TRENDS OF COMPUTATIONAL FLUID DYNAMICS SOFTWARE APPLICATIONS IN CHEMICAL ENGINEERING

The paper presents a brief overview of advanced novel applications and future trends of Computational Fluid Dynamics software in Chemical Engineering. Among the cases of major importance, single phase turbulent flow, as well as multiphase flow models are reviewed. Referring to single phase flows, the LES and RANS approaches are described and illustrated. The RANS approach is revealed as the most popular and inexpensive method for the analysis and solving of technical tasks. The paper reports on two recent modeling applications, namely, the CFD facilitated design of a new mixing impeller, and the CFD characterization of impeller mixing efficiency. Multiphase models of increased sophistication describing solid, liquid and gas flows with simultaneous mass transfer between the phases are summarized with emphasis on their applications to describe evaporation, condensation, as well as chemical reactions in process equipment such as distillation columns and fluidized beds. The future trends and directions in Computer Aided methods for the analysis of Chemical Engineering processes incorporate developments, such as the integration of various pieces of software including flow sheet modeling, CFD modeling and complex reaction and thermodynamic models.

Key words: Fluent, Software, Chemical engineering.

The classical working methods of chemical engineers, which rely heavily on empiricism, practical experience, extensive consultation of printed handbooks, and manual calculations, may no longer be suited for the new and changing environment. A review and discussion of evolution and influence of computational software tools on engineering design and development practice is presented in the study of Bakker et al. [1]. According to this study, the computational tools available to chemical engineers can be classified in three main categories. Flowsheet modeling software can be used to analyze the operation of complete plants. In order to make the models tractable, simplified hydrodynamic models with reduced reaction sets are often used for the individual chemical reactors. On the other end of the spectrum, specialized software exists to model complex chemistry. Such software can handle stiff reaction sets with hundreds of surface and volumetric reactions, but is not suitable to model either complete plants, nor is it able to take the effect of the hydrodynamics of the reactor into account. In between these two extremes falls computational fluid dynamics software, which can model both chemical reactions and the link with reactor hydrodynamics. The field of computational fluid dynamics, or CFD, has grown and changed rapidly during the past twenty years. A number of the components of CFD

technology are examined below. In addition to summarizing the current states in each of these areas, the anticipated trends that are likely to occur in future generations of CFD software are also described.

SINGLE PHASE TURBULENT FLOW

Many exciting physical models have become available in commercial CFD packages in the past decade, and their success and usability are due in part to the increased capabilities of today's computers. For turbulent flows, the large eddy simulation (LES) model is one example. This transient model, which requires a relatively fine mesh, follows mid- to large-scale turbulent eddies as they grow, change, and decay during multiple cycles. The cost of performing a transient calculation of this sort on a fine mesh over many eddy lifetimes was considered prohibitive in past years, but it is now within easy reach on most platforms. It has shed new light on phenomena that have been widely observed, from acoustics to instabilities in flames and stirred tanks.

The RANS approach is, however, still revealed as the most popular and inexpensive method for the analysis and solving of technical tasks. The use of RANS based simulations is now used routinely to assess, compare and understand design modifications to process equipment. The powerful and user-friendly post-processing capabilities of the CFD packages, allow the easier understanding of complex flow patterns and the better communication of scientific and engineering findings between the various parties involved in the product or process design. Two recent modeling applications, namely, the CFD facilitated design of a new mixing impeller and the CFD characterization of impeller mixing efficiency, are examples of this.

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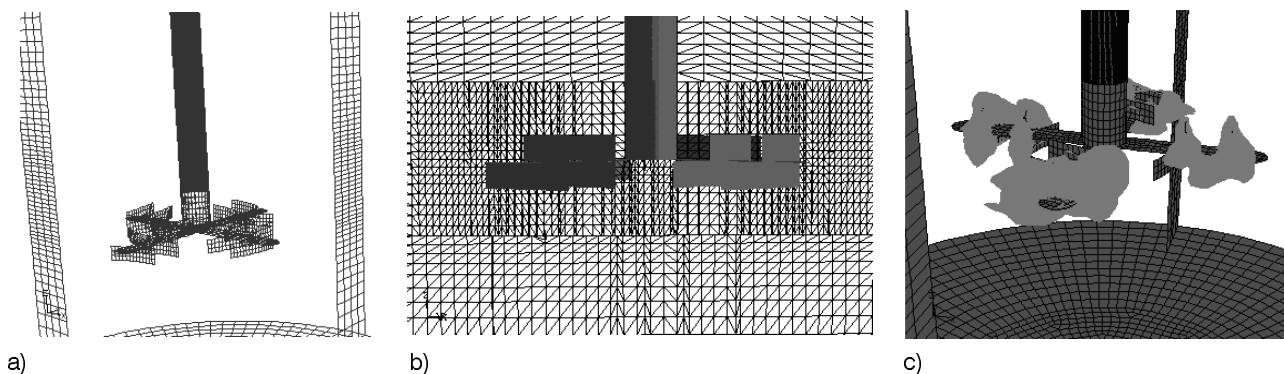


Figure 1. View of the impeller (a) and the mesh (b) at the visualization plane. The mesh consisted of 175 804 cells. (c) The strain rate 500 s^{-1} iso-zone.

CFD facilitated design of a new mixing impeller

CFD allows direct generation of the flow field of a device for mechanical agitation. While generating such complex information, one can easily decide the outcome of an intended design based on the fluid flow advantages and disadvantages obtained. The example is a new geometry flat-blade impeller sketched initially in Sofia Technical University [2] the advantage of which over the conventional type had to be proved. The multivortex device MV comprising multidirectional blades, is shown in Figure 1a and the Figure 1b contains part of the mesh. The Navier Stokes equations for stirred flow coupled with "k- ϵ " turbulence approximation allowed the derivation of some major flow characteristics of this device, e.g. flow pattern diagram, velocity and turbulence intensity contours and iso-zones. The general flow pattern of the device and the spread of the iso-zone of the strain rate 500 s^{-1} are illustrated in Figure 2.

On the basis of this data, the macro parameters of mixing, namely the power number and mixing time were computed and gave the values, presented in Table 1. While comparing some of these data with the parameters of a conventional flat-blade Rushton turbine,

one could infer the positive solution required for the device approval.

The whole procedure of the study took three weeks for developing the mesh and another month to perform. In contrast, bearing in mind the versatility of the information obtained, the experiment would take more than six months and would be rather more expensive.

CFD characterization of impeller mixing efficiency

Impeller mixing efficiency can be represented as mixing time versus input energy. The mixing time quantifies the homogenization rate in single phase flow. It is determined, as the time required to reach 99% uniformity of a mixture starting at zero time and zero concentration before reaching the end equilibrium values C_{∞} . Provided the flow field of the impeller is defined, the concentration field is generated following a pulse tracer input in an inlet point under the liquid surface. The concentration function $C(t)$ is extended-into a measure of the current uniformity degree $U(t)$, as

$$U(t) = 1 - \frac{(C_{\infty} - C(t))}{C_{\infty}}$$

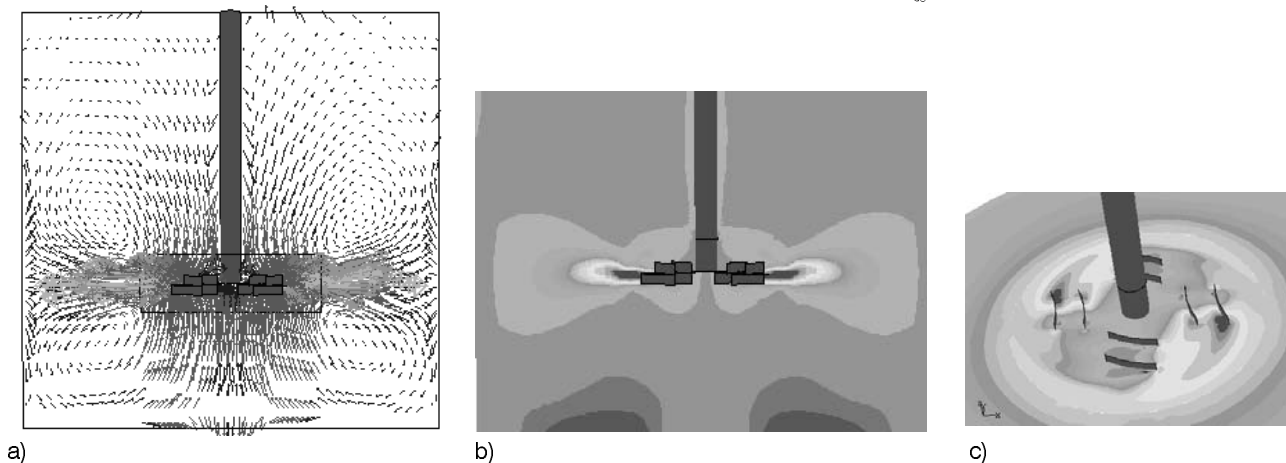


Figure 2. Flow patterns and radial velocity contours for the MV impeller

Table 1. MV vs. conventional turbine predicted values for the power number Po

Case No	System Properties	Po
1	Rushton turbine (RT), water, 600 rpm, 63 648 cells periodic sol'n	5.40
2	RT, water, 600 rpm, 184 944 cells, FLUENT 6.0 Solution	5.45
3	RT, water, 900 rpm, 56 736 cells	4.25
4	Smith turbine, water, 379 760 cells	3.15
5	MV upper blade design, water, 600 rpm, 175000 cells	0,65
6	MV low blade design, water, 600 rpm, 175000 cells	0,37

The method follows the transport of a tracer liquid, similar to dye injection. The tracer is added near the liquid surface, and the concentrations are monitored throughout the vessel as a function of time. The quantity time-99 is determined at various locations in the tank and averaged further to obtain the mixing time t_m . The procedure is illustrated in Figure 2. and Figure 3.

The mixing efficiency is high where the mixing time per unit specific input power is smaller. The final results for several mixing impellers are presented in Table 2.

The task was been solved entirely by computation using the commercial CFD code (FLUENT 6) and the results were delivered as part of an overall characterization of the impeller NS (reported previously by Vlaev et al. in Pennsylvania, USA 2001 [3]).

MULTIPHASE FLOW

The modeling of multiple phases is an area that has seen increased sophistication during the past several years. The general purpose Eulerian multiphase model is now routinely applied for modeling gas-liquid and liquid-liquid mixtures, while its sister, the granular

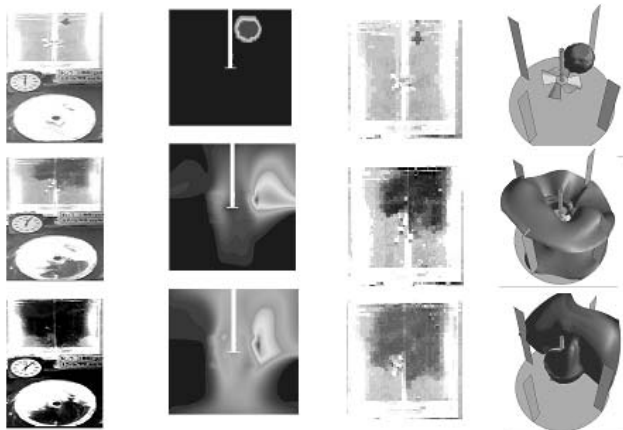


Figure 2. Views at time: 0 s, 3 s, 6 s, 10 s obtained by CFD (b-d) and experimentally (a)

Table 2. Values of mixing time θ_m and power number Po for various impellers

Impeller	Po	Fluid	Tank	U(t)	θ_m (exp)	θ_m (predicted)
NS 25	1,1	Water	300	1.01	22	25 s
NS 25	1,1	Water	300	1.06	22	20 s
NS 45	0,9	Water	400	0.97	6	7.5 s
Rushton	5,4	Water	400	0,99	10	13.5
PBT	1,3		400	0,99	72	61.5

Eulerian multiphase model, has been specifically developed for mixtures containing solids.

The first commercially available multiphase models were been released in the late '90s and were invariably applied on structured 2-dimensional simplified domains, to model the hydrodynamics of isothermal, non-reacting systems (see for example Faltsi-Saravelou et al., [4]).

Multiphase models are now able to describe mixtures of multiple phases of any combination. In addition, mass transfer between phases allows for the simulation of evaporation, condensation, and chemical reactions in multiple phases.

One example of such a recently completed study involves the three dimensional modeling of a rotating fluidized bed coal/lignite/biomass gasifier (D. Sofialidis et al., [5]). The model accounts for the rotation of the kiln walls and mixing blades, multiphase flow modelling of the solid (fuel) and gaseous (mixture of gases) phases, heat transfer between the phases and the heated kiln walls and mass transfer due to chemical reaction between species of different (heterogeneous) phases (drying, devolatilization, and char gasification). Figure 4 shows the three-dimensional geometry of the rotating kiln, while isosurfaces of the solids volume fraction at a series of time intervals are depicted in Figure 5. Dark and light grey surfaces indicate different solid species; the dark one pushing the light one downstream as it continues to be injected in the rotary kiln. The purpose of the study was to arrive at a realistic, industrial-scale kiln geometry and operating conditions, in order to achieve the required residence time for the completion of the solids thermochemical treatment and sufficient mixing.

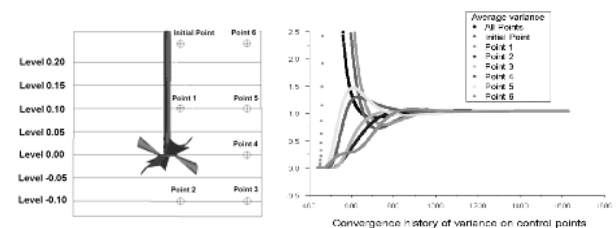


Figure 3. The specific mixing impeller measurement points and relevant concentration evolution to mixing time 900 s

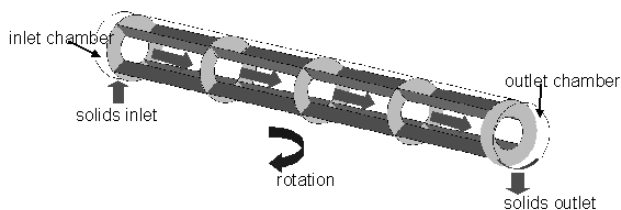


Figure 4. Geometry of the 3D kiln model

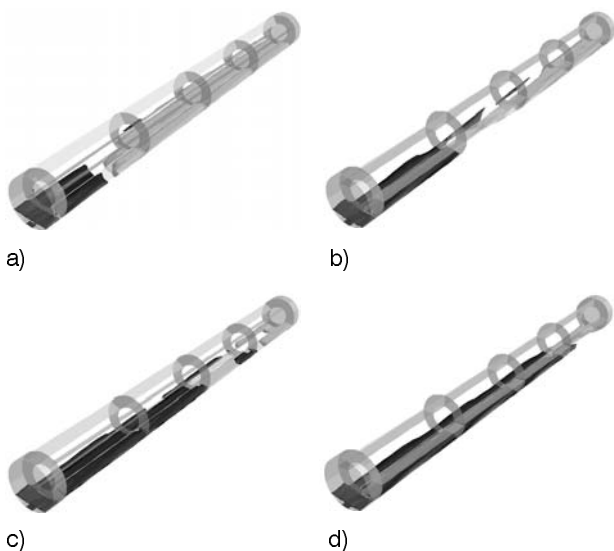


Figure 5. Isosurfaces of the solids volume fraction: (a) $t = 100$ [s], (b) $t = 200$ [s], (c) $t = 300$ [s] and (d) $t = 350$ [s].

Another example, utilizes a different approach for modeling several designs of multiphase flow bioreactors (Kumar Dhanasekharan [6]). Bioreactors are nowadays used to manufacture a wide variety of products, and it is increasingly becoming important to scale-up bioreactors to meet higher demands. Computational approaches based on CFD can be used to simulate and



Figure 6. An airlift reactor has sparged air in the larger (riser) section and circulation through the narrower downcomer. The air-water interface (left), bubble size distribution (middle) and oxygen concentration (right) are shown.

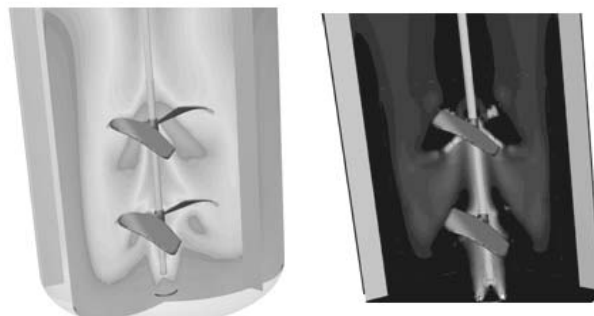
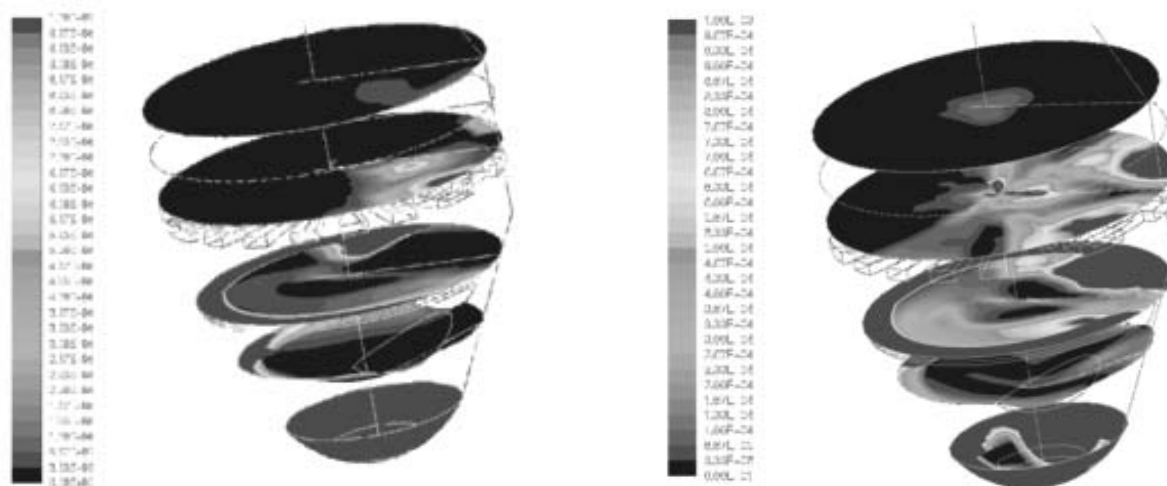


Figure 7. Stirred tank reactors are often used for mammalian cell culture solutions. Bubble size distribution (left) shows small sizes (due to breakup) in the turbulent impeller region. The mass transfer coefficient (right) is non-uniform.

optimize the distribution of gases within the bioreactor, bubble-size distribution, and mass transfer coefficients. Here the solution of population balance equations for bubble number density, with birth and death terms due to breakup and coalescence, was coupled with CFD calculations to predict the bubble size distribution. Figure 6 depicts an airlift reactor, which has sparged air in the larger (riser) section and circulation through the narrower downcomer (the air-water interface, bubble size distribution and oxygen concentration are shown). Stirred tank reactors are often used for mammalian cell culture solutions. Figure 7 shows an example of a CFD model for such a reactor. The bubble size distribution (top) shows small sizes due to breakup in the turbulent impeller region. The mass transfer coefficient (bottom) is non-uniform.

CFD is a powerful tool to obtain a complete view of the real behavior of distillation tower mass and heat transfer units in the best economic way and in a shorter time compared to the trial and error modification to equipments. CFD is also extremely useful in evaluating equipment response to operating condition changes, prior to implementation on the production line. A pioneering CFD simulation of the vacuum distillation tower at a U.S. refinery is presented in the paper by John Krawczyk [7]. The refinery was increasing their capacity and planned to increase the feed to the vacuum distillation tower. The objective of the CFD study was to compute the liquid entrainment inside the distillation tower for a range of feed rates. Figure 8 shows the modelled three dimensional geometry, and the contours of the liquid fraction in the distillation tower for two different feed rates. The simulation confirmed the safe range of operating conditions, for which no internal modifications to the tower were needed.

Another more recent study (Ricardo Pulido et al. [8]), used CFD simulation for obtaining compositional, thermodynamic, hydraulic and flow data in the whole plate in order to evaluate the design. Finally Valmor de Almeida [9] recently reported the first findings of a collaborative project funded by the US Department of Energy, to simulate and optimize different distillation



a) b)
 Figure 8. Contour Plots of Liquid Volume Fraction in the Column

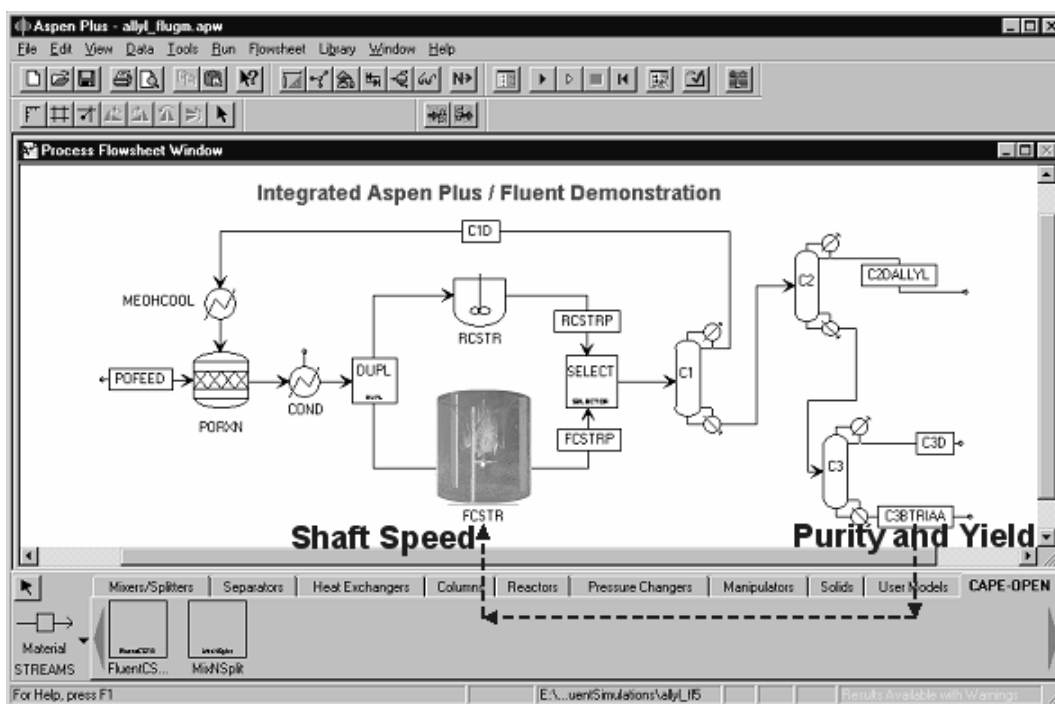


Figure 9. Process flowsheet model linked with a CFD unit operation module

column packing designs. The ultimate goal is to be able to simulate gas-liquid countercurrent flows through as many packing elements as necessary to produce a realistic model of a packed column. Achievement of this goal will show that accurate, large-scale, first-principles simulation of distillation in structured packed columns is finally at hand.

SOFTWARE INTEGRATION

CFD software is usually used to model individual plant components and not the whole process at once. When tied to flowsheet modeling software, however, it

can provide more accurate flow field data (averaged velocities or temperatures) about unit operations than the simplified assumptions normally used for input (Figure 9).

Indeed, the current trend is to integrate these various pieces of software. The flowsheet model uses its standard models for non reaction-critical components such as pipelines, pumps, conveyors, etc. For the critical reaction components, an advanced CFD model automatically replaces the one dimensional models currently included in the flowsheet software. The CFD software automatically exchanges the required data with the flowsheet model. It models both the fluid dynamics

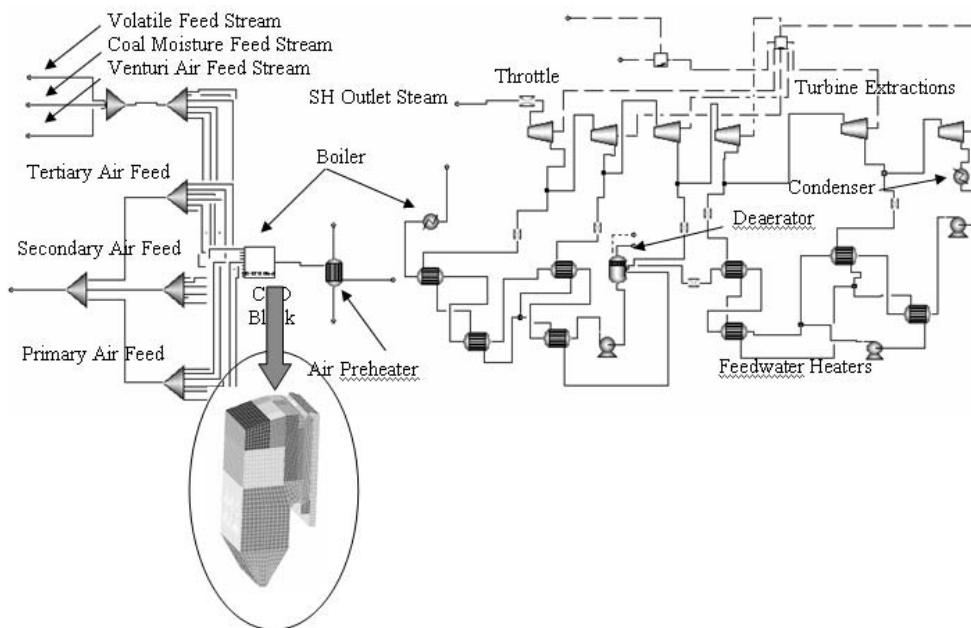


Figure 10. Shows a three-dimensional CFD boiler module integrated into the flowsheet of a steam plant.

of the reactor and the chemical reaction process. For very complex reaction sets, the CFD software may automatically call a specialized chemical reaction program that replaces its standard chemical reaction solver and solves the complex reaction set for every cell in the CFD domain at every fluid flow time step.

Some integrated systems have recently become commercially available and many have been implemented on a custom basis. It is expected that within a few years, software will be commonly available that includes flowsheet modeling, reactor hydrodynamics modeling and fully integrated complex reaction models.

The interoperability and seamless communication of various software components naturally requires the development of communication standards. The CAPE-OPEN Laboratories Network (CO-LaN) [10] is the internationally recognized, user-driven organization for the management of the CAPE-OPEN (CO) standard. The standard defines rules and interfaces that allow CAPE (Computer-Aided Process Engineering) applications or components to interoperate. An example of a process-simulation/CFD package that exploits the CAPE-OPEN standard unit operation interfaces is the FLUENT CFD / Aspen Plus flowsheet interface. In that sense, Fluent is a CO-compliant unit operation that plugs into the Aspen Plus CO Simulation Environment (COSE). It is called automatically and repeatedly as part of the Aspen Plus solution process. Stream information, physical properties, and reaction stoichiometry and parameters are automatically transferred from Aspen Plus to Fluent. Examples of co-simulation cases are presented in (Stephen E. Zitney et al, [11]). Figure 10. shows a three-dimensional CFD boiler module integrated into the flowsheet of a steam plant.

The integration of complex reaction modeling software into CFD packages has recently been made available commercially. For example the CHEMKIN software suite can be linked to the FLUENT CFD package and allows the CFD analysis to use any level of gas-phase or surface kinetics detail in the complex-flow simulations. An example of such a simulation shown in Figure 11, is the simulation of the catalytic oxidation of CH₄ on Pt in a monolith channel for a two-stage gas-turbine combustor [12].

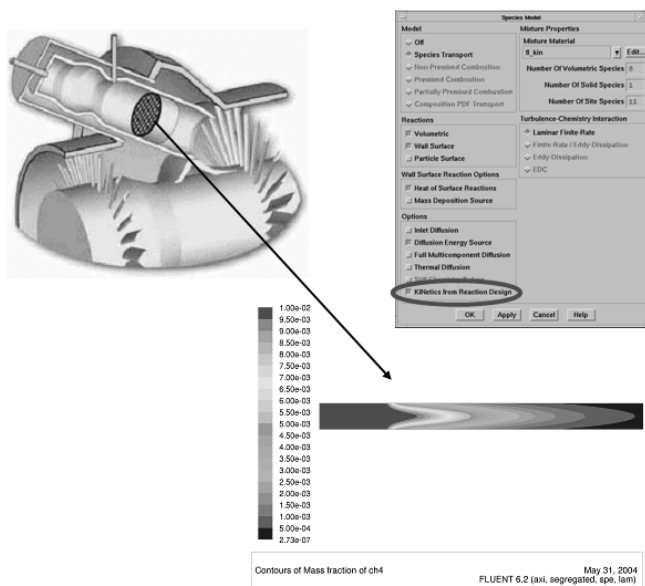


Figure 11. FLUENT/KINETICS simulation of the catalytic oxidation of CH₄ on Pt in a monolith channel for a two-stage gas-turbine combustor

FUTURE TRENDS

The future will most likely bring new approaches to multiphase modeling, in addition to more complex physics (for near-wall modeling or interphase turbulence transfer, for example) and improved numerics. Many models are currently in development and will be available for general use during the next few years. These include crystallization, with sub-models for the onset of nucleation [13], plasma models that couple to gaseous flows [14] and the ability to model micro- and nano-scale phenomena [15]. The introduction of these models will expand the forefront of CFD modeling into many new application areas during the next decade.

As the range of applications where high end computational techniques such as CFD are employed increases, and the time required to achieve the numerical solutions shortens, commercial CFD vendors are also focusing on making the advanced software simulation technology also available to non-experts. Efforts are concentrated to develop simple wizard-like interfaces and web portals for allowing use-on-demand of the software.

REFERENCES

- [1] André Bakker, Ahmad Haidari, Elizabeth M. Marshall, "Chemical Reaction", TECHNICAL NOTES TN159, Fluent Inc., 10 Cavendish Court, Centerra Resource Park, Lebanon, NH 03766, 2001.
- [2] Kraitchev, S., S.D. Vlaev, V. Lossev, P. Staykov, A new arc-blade version of a turbine impeller suitable for bioreactors, *Biotechnol. Equipment* **15** (2001), 128-131.
- [3] Vlaev, S.D., P. Staykov, R. Mann, H. Hristov, P. Mavros. Experimental and CFD Characterisation of a New Energy-Saving Fluid-Foil Mixing Impeller for the Process Industry, Paper at Mixing XVIII 18th Biennial Conf. NAMF, June 24/29, 2001, Pennsylvania, USA.
- [4] O. Faltsi-Saravelou, D. Koufos, D. Cokljat and P. Wild, "CFD Modeling of a Two-Phase FBR", *Two-Phase Flow Modeling and Experimentation*, 1999, Eds. G.P. Celata, P. Di Marco, and R.K. Shah, Proceedings of the Second International Symposium on Two-Phase Flow Modeling and Experimentation, Rome, Italy, 23-26 May, 1999.
- [5] D. Sofialidis, O. Faltsi, K. Sardi, G. Skevis, G. Skodras, S. P. Kaldis and G. P. Sakellariopoulos, "Modeling Low-Temperature Carbonization of Solid Fuels in a Heated Rotary Kiln for Clean Fuel Production", *Fuel*, In press, 2005.
- [6] Kumar Dhanasekharan, "Design and Scale-Up of Bioreactors Using Population Balance and CFD", *Journal Article, JA-218*, Fluent Inc, 10 Cavendish Court, Centerra Resource Park, Lebanon, NH 03766, 2004
- [7] John Krawczyk (2001) "Multiphase CFD Models of a Vacuum Distillation Tower" *Proceedings, Fluent Users Group Meeting*, 2001.
- [8] Ricardo Pulido, Yi Dai, Leodegario Monroy, "Process and CFD Simulations of a Section of a Pilot Plant Distillation Tower" *TECHNICAL NOTE TN-251*, Fluent Inc, 10 Cavendish Court, Centerra Resource Park, Lebanon, NH 03766, 2004.
- [9] Valmor de Almeida, Rafiqul Khan and David Schowalter, "Realistic Distillation Modeling" *Fluent NEWS* spring 2004, Fluent Inc., 10 Cavendish Court, Centerra Resource Park, Lebanon, NH 03766, 2004.
- [10] http://www.colan.org/COLAN_2003_Leaflet.pdf
- [11] Stephen E. Zitney, Madhava Syamial, Ahmad H. Haidari, "Integration of CFD and Process Simulation for Improved Reactor Design", *AIChE 2001 Annual Meeting*, Reno, NV, November 4-9, 2001.
- [12] http://www.chemkin.com/company/open_archive/news_20041118.html.
- [13] Kumar M. Dhanasekharan, "Solution Crystallization with FLUENT", *Proceedings Fluent Users Group Meeting*, 2003.
- [14] Balaji Devulapalli and Gabriel Font, "Etching of Silicon Dioxide using C4F8 Discharges in a Plasma Reactor", *Proceedings Fluent Users Group Meeting*, 2001.
- [15] S.R. Deshmuch and G. Vlachos, "The Power of Microreactors", *Fluent NEWS* Summer 2005, Fluent Inc., 10 Cavendish Court, Centerra Resource Park, Lebanon, NH 03766, 2005.

IZVOD

NOVA POLJA I BUDUĆI PRAVCI PRIMENE KOMPJUTERIZOVANE DINAMIKE FLUIDA U HEMIJSKOM INŽENJERSTVU

(Pregledni rad)

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U radu se analiziraju neka nova polja i budući pravci primene kompjuterizovane dinamike fluida (CFD) u hemijskom inženjerstvu. Analiziraju se neke najvažnije primene ovog softvera: turbulentnog strujanje fluida i strujanje kod višefaznih sistema. U prvom slučaju su detaljnije opisane i prikazane primene LES i RANS programa. Takođe se prikazuje mogućnost primene CFD programa za projektovanje i određivanje optimalnog tipa mešalice. U drugom slučaju se analizira tok čvrste faze, tečnog i gasovitog fluida uz istovremen prenos mase između faza kod operacija isparavanja, kristalizacije ili hemijske reakcije (destilacione kolone, reaktori sa fluidizovanim slojem čvrste faze). Ukazano je da razvoj primene CFD u višefaznim sistemima mora da bude praćen razvojem drugih programa i modela koji se mogu povezati sa osnovnim CFD modelom (razvoj tehnološke šeme, razvoj kompleksnih modela koji uključuju analizu karakteristične hemijske reakcije i termodinamike tj. stanja fluida).

Ključne reči: FLUENT, Softveri, Hemijsko inženjerstvo.