초고속·대용량 Computing에 기반한 폭발 Modeling 및 Simulation의 발전방향

원동빈, 신동일[1,*]
명지대학교 화학공학과, [1]명지대학교 화학공학과・화재공학과
(dongil@mju.ac.kr[*])

Advances in Explosion Modeling and Simulation Based on the High Speed, Large Scale Computing

Dong Bin Won, Dongil Shin[1,*]
Department of Chemical Engineering, Myongji University
[1]Departments of Chemical Engineering and Fire Engineering, Myongji University
(dongil@mju.ac.kr[*])

1. Introduction

Despite significant improvements in process safety technology and process safety management, fires and explosions are still the dominant cause for the largest losses in the chemical and petroleum industry [6]. The burden of fire safety related activities on western industrialized economies has been estimated (by Snell and by Richardson) to be between 0.6% and 1% of GDP. The magnitude of this cost in an increasingly competitive global economy is unsustainable [3].

Fire and explosion modeling can be accomplished through the use of experimental or mathematical techniques. Experimental methods include such methods as reduced and full-scale replicas of the situation or phenomenon being studied [9]. Mathematical models are commonly divided into two groups: stochastic and deterministic models. Stochastic models treat fire growth as a sequence of events or steps. The events, coupled with their probabilities, are used to predict the progress of a fire. Deterministic models predict fire development based on the solution of mathematical equations that describe the physical and chemical behavior of fire.

Time-accurate, full physics simulations of accidental fires and explosions require consideration of fundamental gas and condensed phase chemistry, structural mechanics, turbulent reacting flows, convective and radiative heat transfer, and mass transfer [5,11]. It is also required to model the physical complexities from the molecular level of high energy materials, through millimeter-sized representations of the container, to the meter-sized representations of the fire spread. Due to the inherent multiple scales [13], the spatial requirements may exceed the terabyte range for the full simulation. The computation will also require 10^{10} time-steps to compute the physical time scales ranging from microseconds to minutes or hours [12].

Through the brief review of recent progresses in modeling and simulation of fires and explosions, we are focused on providing science-based tools for the numerical simulation of accidental fires, especially within the context of handling and storage of hydrocarbons. The application of quantum mechanics and molecular simulation methods can yield new insights into the thermal reactivity of large molecules and nanoscale structures. We are also investigating the coupling of the micro-scale and meso-scale contributions to the macroscopic application in order to provide full-physics accuracy and the effective utilization of the Grid computing environment and consisting supercomputers. The Computational and Access Grids may provide a long-waited computational infrastructure that can support multiphysics modeling of large-scale, complex phenomena and interactive collaboration among distributed sites.

2. Numerical Modeling and Simulation of Fire and Explosion: Adoption of Large-Scale Computations

2.1 Direct Numerical Simulation (DNS)

This methodology is the only truly fundamental theoretical approach and its use has already contributed to improving subsets of other models. Solving the Navier Stokes equations which govern fluid flow without averaging is the most accurate approach to turbulence. In this approach the whole range of length and time scales are solved, without any modeling approximation [4]. The accuracy of this method makes it a very powerful tool for approaching turbulent flow and an important basis for the more complex problem of reactive turbulent flow. Chemistry is usually incorporated by look-up approaches or more complex chemical models run externally.

The inhibition to its wide adoption is the large computer source requirement. This places a restriction on the size of geometry which can be tackled. Given current computer resources DNS is not now a successor to other engineering tools. Its current usefulness resides in the large amount of detail that can be obtained about a turbulent flow field. The detailed time and space resolution which DNS calculations give exceed in many respects even the detailed data acquired by all but the most highly and intensively instrumented experiments. They, therefore, give truly new insight into the physics of the processes involved. Direct Numerical Simulation is also an important tool in getting the most out of existing experimental databases [4].

2.2 Fire Dynamics Simulator of NIST

The current state of the art in computer fire modeling is exemplified by National Institute of Standards and Technology (NIST)'s latest contribution to fire modeling, the Fire Dynamics Simulator (FDS). FDS is a computational fluid dynamics (CFD) model of fire-driven fluid flow. The software solves numerically a form of the Navier-Stokes equations appropriate for low-speed, thermally-driven flow with an emphasis on smoke and heat transport from fires. The downside is that CFD calculations can easily take days to run since they solve for many variables in each of hundreds of thousands or even millions of grid cells [7]. Smokeview is a visualization program that is used to display the results of an FDS simulation.

2.3 Center for the Simulation of Accidental Fires and Explosions (C-SAFE)

The C-SAFE at the University of Utah focuses on providing state-of-the-art, science-based tools for the numerical simulation of accidental fires and explosions, especially in the context of handling and storing highly flammable materials [8,12,13]. C-SAFE will provide a scalable, high-performance problem solving environment (PSE) in which fundamental chemistry and engineering physics are fully coupled with nonlinear solvers, optimization, computational steering, visualization, and experimental data verification. The availability of simulations using this system will help to better evaluate the risks and safety issues associated with fires and explosions. Fig. 1 shows the research and development roadmap of C-SAFE.

2.4 FireGrid

In the UK, the recent Independent Review of the Fire Service highlighted the need for modernization. Among other things, the Review envisaged the future Fire Service having the capacity and resilience to respond to major incidents of terrorism, as well as other emergencies, with much greater efficiency. The FireGrid (see Fig. 2) concept will use Grid technology, advanced sensor networks and high performance computing to make this vision become reality

[3].

In FireGrid's "Emergency Response" mode, parallelization and on-demand Grids will allow the Computational Fluid Dynamics (CFD) fire models and Finite Element (FE) structural models to be run faster than real time. Pre-deployed sensors and wireless networks will obtain data from the burning building which will be used to guide and accelerate the computations. Data from the computations and sensors will be input to the real-time planner. Conventionally, research based on experiments and computational modeling have been considered to be separate activities. FireGrid offers an opportunity to draw the two methodologies together in order to gain special insights into problems that would not be possible using one or the other in isolation.

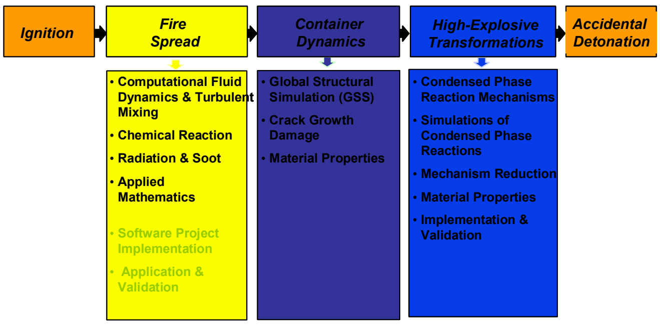

Fig. 1 The main roadmap of C-SAFE [8]

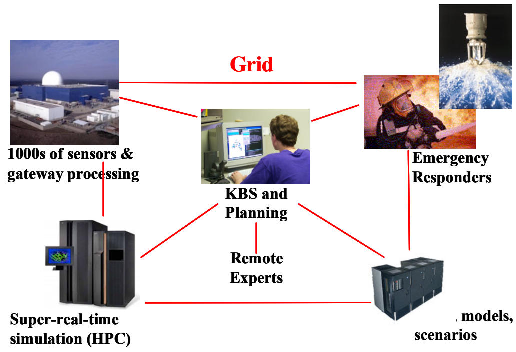

Fig. 2 FireGrid vision [3]

3. Grids: Advanced Environment for Large-Scael Computation and Collaboration

High performance computing technology is of great importance in modem industry and science. For instance, scientists seek new drugs for cancer or AIDS by using supercomputers. Engineers design new automotive and aircraft through computer simulations. However, ever with a 100GFlops supercomputer, scientists still need a faster computer. There are always more complex problems which can not be solved by the most powerful computer in the world. Grid technology offers a solution to this problem. The term Grid stems from the analogy with an electricity grid. Computers, data storages and other scientific facilities are connected by Grid technology. They form a huge computing resource, data repository and virtual experimental laboratory.

Nowadays, in many advanced and developing countries, Grid technology has become the hottest issue. The K*Grid project is an initiative in Grid researches supported by the Ministry of Information and Communication in Korea [10]. The main goal of K*Grid project is to provide an extremely powerful research environment to both industries and academia. A huge amount of computing power, virtual experiment facilities and international collaborations would be available via the K*Grid. The K*Grid project includes the development of national Grid infrastructure and Grid middleware, and the main research topics are in scientific applications and essential software development. Supercomputers and high performance clusters are being connected to the Grid infrastructure, including various resources in the Asia Pacific.

The Access Grid®is an ensemble of resources including multimedia large-format displays, presentation and interactive environments, and interfaces to Grid middleware and to visualization environments [1]. These resources are used to support group-to-group interactions across the Grid. For example, the Access Grid (AG) is used for large-scale distributed meetings, collaborative work sessions, seminars, lectures, tutorials, and training. The Access Grid thus differs from desktop-to-desktop tools that focus on individual communication.

4. 8iConclusion

e-Science is offering a new opportunity to significantly improve the fire and explosion-related research and the intervention in emergencies involving fires and explosions. In contrast to large outdoor fires, industrial fires are usually much more highly localized but intense emitters of heat, smoke, and other combustion products. This is particularly true if the fuel is a petroleum based substance, with a high energy density and sooting potential [2]. This paper discussed the research challenges and our approach to solving them, especially related to applying molecular simulation and large-scale computational techniques to gain advanced theoretical insights into accidental fires and explosions. Developing the proposed system and extensively using it through the cooperation in the interesting parties will help better evaluate the risks and safety issues associated with fires and explosions in involving countries.

Acknowledgment

This work was partially supported by the Korea Research Foundation Grant funded by Korean Government (R08-2003-000-10982-0).

References

[1] *Access Grid home page* (2005). http://www.accessgrid.org

[2] Baum, H. R. and K. B. McGrattan (1999). Simulation of large industrial outdoor fires, *Proc. 6th International Symposium of International Assoc. for Fire Safety Sci.*

[3] Berry, D., A. Usmani, J. Torero, A. Tate, S. McLaughlin, S. Potter, A. Trew, R. Baxter, M. Bull and M. Atkinson (2005). *FireGrid: Integrated emergency response and fire safety engineering for the future built environment*, http://www.firegrid.org

[4] Bull, D. C. (2004). *A critical review of post Piper-Alpha developments in explosion science for the Offshore Industry*, HSE Books, U.K.

[5] Cant, R. S., W. N. Dawes and A. M. Savill (2004). Advanced CFD and modeling of accidental explosions, *Annu. Rev. Fluid Mech.*, **36**, 05.1-05.23.

[6] Crowl, D. A. and J. Louvar (2002). *Chemical Process Safety—Fundamentals with Applications*, 2nd Ed., Prentice-Hall.

[7] Forney, G. P., D. Madrzykowski, K. B. McGrattan and L. Sheppard (2003). Understanding fire and smoke flow through modeling and visualization, *IEEE Computer Graphics and Applications*, July/August, 6-13. http://fire.nist.gov/fds/

[8] Henderson, T. C., P. A. McMurtry, P. J. Smith, G. A. Voth, C. A. Wight and D. W. Pershing (2000). Simulating accidental fires and explosions, *Computing in Science and Engineering*, March/April, 64-76.

[9] Janssens, M. L. (2000). *An Introduction to Mathematical Fire Modeling*, 2nd Ed., Technomic Publishing Co., Lancaster, PA.

[10] *K*Grid home page* (2005). http://www.gridcenter.or.kr

[11] Lea, C. J. and H. S. Ledin (2002). A review of the state-of-the-art in gas explosion modelling, *Health & Safety Laboratory Report*, HSL/2002/02.

[12] Smith, P. J. (2005). *Incorporating microscopic information in macroscopic fire simulations*. http://www.csafe.utah.edu

[13] Violi, A., A. F. Sarofim and G. A. Voth (2004). Kinetic Monte Carlo-Molecular Dynamic Approach to Model Soot Inception, *Combust. Sci. and Tech.*, **176**, 1-14.