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# KIVA

## KIVA Software

QUOTE: “We are finding it [KIVA] quite accurate for simulating air jets and air -mist water sprays. The modeling results on free air-mist agree very well with experimental ones and the predictions concerning impinging mists look very encouraging. I believe KIVA will be very useful for understanding and improving spray cooling in steel continuous casting.”

*A. Humberto Castillejos E., Ph.D., Prof. of Metallurgical Engineering at Centro de Investigación y de Estudios Avanzados del IPN*

Fuel economy is heavily dependent upon engine efficiency, which in turn depends to a large degree on how fuel is burned within the cylinders of the engine. Higher in-cylinder pressures and temperature lead to increased fuel economy, but they also create more difficulty in controlling the combustion process. Poorly controlled and incomplete combustion can cause higher levels of emissions and lower engine efficiencies.

One of the goals of U.S. and foreign automakers and engine manufactures is to optimize combustion engines with the objective of reducing fuel usage, retaining or increasing power, and reducing undesirable emissions.

In order to optimize combustion processes, engine designers have traditionally undertaken manual engine modifications, conducted testing, and analyzed the results. This iterative process is painstaking slow, costly, and does not lend itself to identifying the optimal engine design specifications.

In response to these problems, Los Alamos National Laboratory (LANL) scientists have developed KIVA, an advanced computational fluid dynamics (CFD) modeling code that accurately simulates the in-cylinder processes of engines.

KIVA, a transient, three-dimensional, multiphase, multicomponent code for the analysis of chemically reacting flows with sprays has been under development at LANL for many years. The code uses an Arbitrary Lagrangian Eulerian (ALE) methodology on a staggered grid, and discretizes space using the finite-volume technique. The code uses an implicit time-advancement with the exception of the advective terms that are cast in an explicit but second-order monotonicity-preserving manner. Also, the convection calculations can be subcycled in the desired regions to avoid restricting the time step due to Courant conditions.

KIVA's functionality extends from low speeds to supersonic flows for both laminar and turbulent regimes. Transport and chemical reactions for an arbitrary number of species and their chemical reactions is provided. A stochastic particle method is used to calculate evaporating liquid sprays, including the effects of droplet collisions, agglomeration, and aerodynamic breakups.

Although specifically designed for simulating internal combustion engines, the modularity of the code facilitates easy modifications for solving a variety of hydrodynamics problems involving chemical reactions. The versatility and range of features have made KIVA programs attractive to a variety of non-engine applications as well. These range from convection towers to modeling silicon dioxide condensation in high pressure oxidation chambers. Other applications have included the analysis of flows in automotive catalytic converters, power plant smokestack cleaning, pyrolytic treatment of biomass, design of fire suppression systems, pulsed detonation propulsion systems, stationary burners, aerosol dispersion, and design of heating, ventilation, and air conditioning systems. The code has found a widespread application in the automotive industry.

KIVA is a family of Fortran-based Computational Fluid Dynamics (CFD) software that predicts complex multi-species multi-phase turbulent fuel and air flows. KIVA models all engine combustion processes with models for spray, soot formation, spark ignition, and reactive chemistry (including pollutant-

formation processes). Employing KIVA software helps to optimize internal combustion engine processes, including diesel engines, for higher efficiency and lower emissions. KIVA engine modeling routines such as spray and core CFD Arbitrary Lagrangian-Eulerian (ALE) algorithms are now ubiquitous in the industry of engine code simulators. In addition, many engineers and researchers have made modifications to or enhanced our routines to address specific problems in engine designs.

This software is ever evolving and continues building from its origins. The software team is constantly employing the newest algorithms, numerical methods, and models in response to industry needs. Each version has added significant elements to the previous licensed version; with the current progression changing the entire numerical method to the state-of-the-art for CFD modeling, known as KIVA-hpFE, a finite element based method. LANL researchers recently developed KIVA-4mpi, a parallel version of KIVA-4. This software also solves chemically reacting, turbulent, multi-phase viscous flows, but does this on multiple computer processors with a distributed computational domain (grid).

Currently, Los Alamos National Laboratory licenses KIVA-3V, KIVA-4, and KIVA-4mpi source code through a nonexclusive, nontransferable end user license agreement for a reasonable licensing fee. A demo version is also available and can be accessed online. The demo version has been downloaded more than 600 times since January 2012.

### **KIVA-3V**

KIVA-3V is the most mature version of KIVA still maintained and distributed through LANL; it is an improved version of the earlier Federal Laboratory Consortium Excellence in Technology Transfer Award-winning KIVA3 (1993), extended to model vertical or canted valves in the cylinder head of a gasoline or diesel engine. KIVA3, in turn, was based on the earlier KIVA2 (1989) and used the same numerical solution procedure and solved the same types of equations.

KIVA-3V uses a block-structured mesh with connectivity defined through indirect addressing. The departure from a single rectangular structure in logical space allows complex geometries to be modeled with significantly greater efficiency because large regions of deactivated cells are no longer necessary. Cell-face boundary conditions permit greater flexibility and simplification in the application of boundary conditions. KIVA-3V also contains a number of significant improvements over its predecessors. New features enhanced the robustness, efficiency, and usefulness of the overall program for engine modeling. Automatic restart of the cycle with a reduced time step in case of iteration limit or temperature overflow effectively reduced code crashes. A new option provided automatic deactivation of a port region when it is closed from the cylinder and reactivation when it communicates with the cylinder. Extensions to the particle-based liquid wall film model made the model more complete and a split injection option was also added. A new subroutine monitors the liquid and gaseous fuel phases and energy balance data and emissions are monitored and printed. In addition, new features were added to the LANL-developed grid generator, K3PREP, and the KIVA graphics post processor, K3POST.

### **KIVA-4**

KIVA-4 is maintained and distributed through LANL. While KIVA-4 maintains the full generality of KIVA-3V, it adds the capability of computing with unstructured grids. Unstructured grids can be generated more easily than structured grids for complex geometries. The unstructured grids may be composed of a variety of elements including hexahedra, prisms,

pyramids, and tetrahedra. However, the numerical accuracy diminishes when the grid is not composed of hexahedra.

KIVA-4 was developed to work with the many geometries accommodated within KIVA-3V, which includes 2D axisymmetric, 2D planar, 3D axisymmetric sector geometries, and full 3D geometries. KIVA-4 also features a multicomponent fuel evaporation algorithm. Many of the numerical algorithms in KIVA-3V generalize properly to unstructured meshes; however, fundamental changes were needed in the solution of the pressure equation and the fluxing of momentum. In addition, KIVA-4 loops over cell faces to compute diffusion terms.

### **KIVA-4mpi**

Recently, LANL researchers developed KIVA-4mpi, a parallel version of KIVA-4, and the most advanced version of KIVA maintained and distributed by LANL. KIVA-4mpi also solves chemically reacting, turbulent, multi-phase viscous flows, but does this on multiple computer processors with a distributed computational domain (grid). KIVA-4mpi internal combustion engine modeling capabilities are the same as that of KIVA-4, and are based on the KIVA-4 unstructured grid code. The software is well suited for modeling internal combustion engines on multiple processors using the message passing interface (MPI).

On August 9, 2011, LANL honored the authors of KIVA-4mpi with the Distinguished Copyright Award for demonstrating a breadth of commercial applications, potential to create economic value, and the highest level of technical excellence.

### **KIVA-4 executable version**

KIVA-EXEC is a free, reduced-functionality executable-only trial version of KIVA-4. KIVA-EXEC has all the performance of Los Alamos National Laboratory's premier KIVA-4 code, but with a 45K cell limitation.

KIVA-EXEC is perfect for beginners who do not need or intend to modify the source code.