

1999

## Can KIVA Accurately Simulate a Gas Turbine Combustor?

John R. Rice  
*Purdue University, jrr@cs.purdue.edu*

Report Number:  
99-008

---

Rice, John R., "Can KIVA Accurately Simulate a Gas Turbine Combustor?" (1999). *Department of Computer Science Technical Reports*. Paper 1439.  
<https://docs.lib.purdue.edu/cstech/1439>

This document has been made available through Purdue e-Pubs, a service of the Purdue University Libraries.  
Please contact [epubs@purdue.edu](mailto:epubs@purdue.edu) for additional information.

**CAN KIVA ACCURATELY SIMULATE  
A GAS TURBINE COMBUSTOR?**

**John R. Rice**

**Computer Sciences Department  
Purdue University  
West Lafayette, IN 47907**

**CSD-TR #99-008  
March 1999**

# Can KIVA Accurately Simulate a Gas Turbine Combustor?

John R. Rice\*  
Computer Sciences Department  
Purdue University, West Lafayette, In, 47907, USA

May 5, 1999

## Abstract

KIVA is a widely used code for combustion simulation in engines. We discuss its shortcomings in approximating real gas turbine combustors and what might be done to improve its performance. It is assumed that the combustion and CFD phenomena are modeled with complete accuracy and that the solution of discretized versions of these models is also accurate. Thus the focus is on the geometry, grid systems and structural components. We conclude that KIVA is unlikely to produce reasonably accurate simulations (e.g.,  $\pm 25$ -50%) with reasonable computational effort.

## 1 Introduction

KIVA [1] is a simulation code for internal combustion engines (primarily diesel) that is in world-wide use. Its structure allows it to be adapted to simulate gas turbine combustion. KIVA uses simple numerical and geometric modeling techniques for rather complex physical models of the fluid flows and combustion processes. The focus of this report is on limitations in accuracy and computational efficiency imposed by the simple numerical and geometric modeling. We first present a brief summary of the numerical and geometric modeling techniques in KIVA. In Section 3 we describe realistic combustors and then present in Section 4 a simplified model of them that can be analyzed by 2-dimensional methods. Even though this simplified model is much easier to simulate, we see by the analysis of Section 5 that serious limitations arise in using KIVA. Section 6 discusses how interface relaxation could reduce the limitations due to the grid structure used in KIVA. Interface relaxation probably can be used with modest effort (compared to re-implementing KIVA) and it could provide improved efficiency plus some natural parallelism.

---

\*This work is supported by Dept. of Energy ASCI-ASAP grant LG-6982.

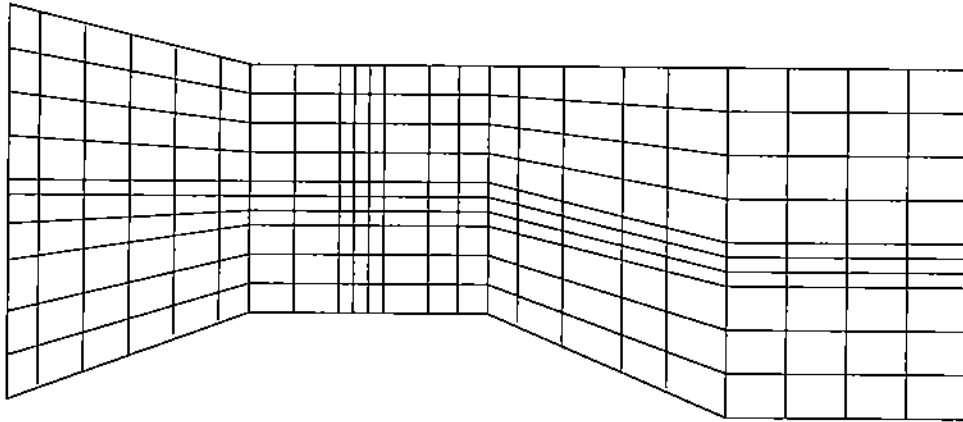


Figure 1. Example 2-dimensional, piecewise linear and uniform size grid on a domain. Within a domain the grid is fitted to a piecewise linear boundary and joins up as a tensor product.

## 2 KIVA Properties

KIVA models the flow and combustion by a set of partial differential equations (PDEs) that includes most (all?) of the important physical phenomena in a combustor. These PDEs are discretized using what we call a *composite, piecewise uniform and linear block grid*. This nonstandard term is illustrated in Figure 1 and the 2-dimensional case where the domain consists of blocks that join up along interfaces. A block can be a single grid wide wide which allows fitting a curved boundary by a broken line approximation. The grids on these interfaces match continuously. KIVA allows several domains to be joined together while maintaining grid continuity but allowing the number of grid lines to change. Figure 2 shows a simple example of three domains joined this way. These two figures illustrate how the grid lines join up continuously and how this affects the spacing of the grids.

KIVA allows the usual boundary conditions for CFD flows. For example, inlet and outlets of the combustor would have the velocity vector, pressure, temperature and mass of the flow specified. Other conditions related to combustion (e.g., fuel flow) can also be specified. Along structural boundaries one also can specify the usual flow conditions.

The PDEs modeling the flow and combustion are discretized by a volume method that resembles both finite elements and finite differences on grids such as those shown in Figures 1 and 2. The resulting linear (or nonlinear) equations are then solved by an explicit time marching procedure. In this study we assume that the PDEs are correct and that the discretized equations are solved properly. Within KIVA it is common to distinguish three types of domains:

- Two phase flow: fuel exists in both liquid and vapor form.

- Combustion: fuel is completely vaporized and combustion takes place.
- Non-combustion: fuel vapor is not present.

This distinction is not important for the study in this report and the transition between types can be made gradually by varying the functions associated with appropriate terms in the PDEs.

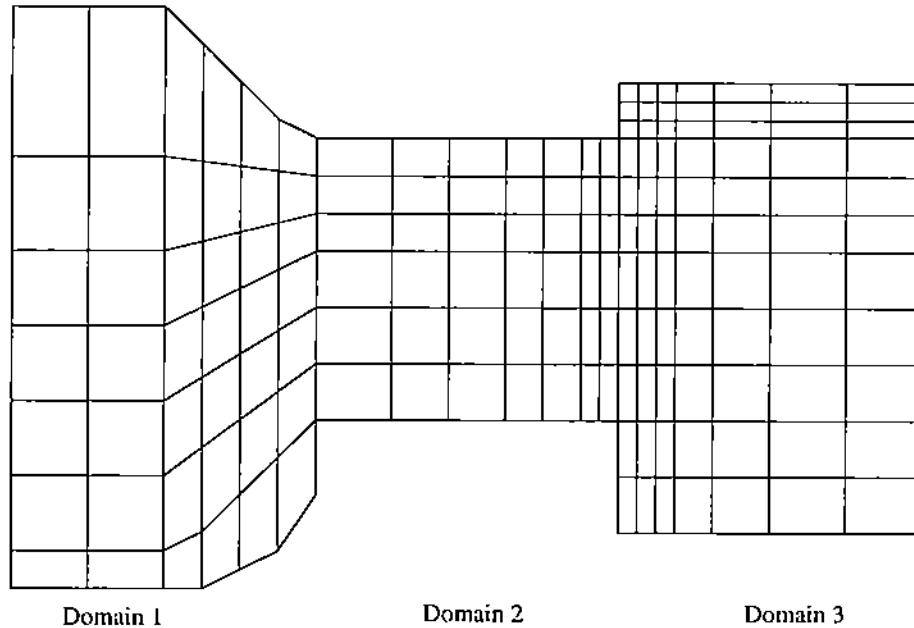
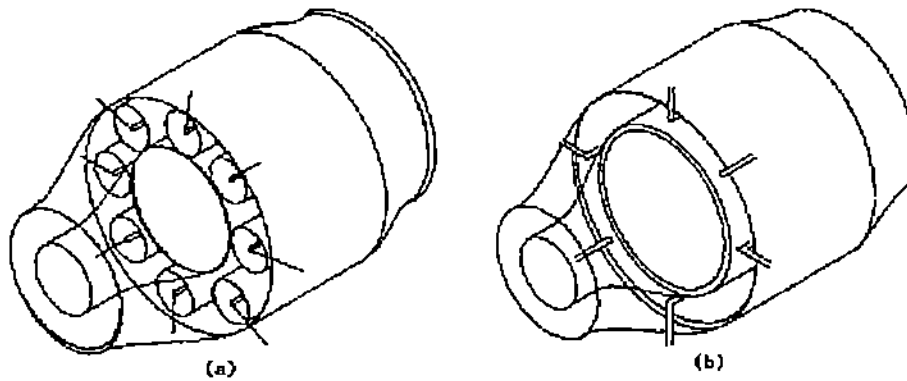


Figure 2. Example of three domains joined in KIVA with continuous grid lines allows for corners in the boundary.

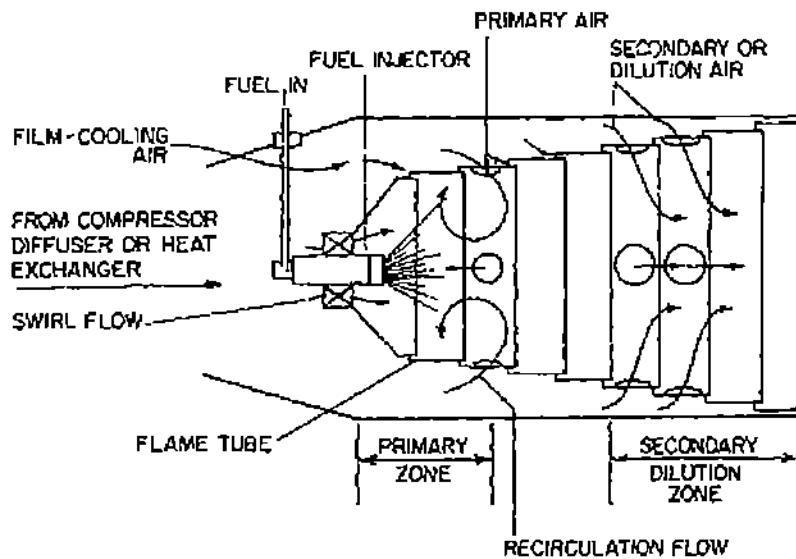
### 3 Gas Turbine Combustors

Figure 3 shows a schematic of two common types of turbine combustors. A turbine engine has approximate cylindrical symmetry with a central shaft area surrounded by gas flow. The gas flow can have several combustor “cans” as shown in Figure 3(a) or be a continuous region with several fuel injectors as in Figure 3(b). Figure 4 shows a schematic of the general form of a combustor and Figure 5 shows a rough sketch of the actual geometry of a can. The principal features to note are (i) the air flow takes several paths which are designed to keep the turbine walls cool enough while supplying just the right amount of oxygen at the right places to burn the fuel efficiently. In the primary zone the flow is deliberately made to swirl in the area of the fuel injection and spray. In the secondary zone more air is introduced to dilute the mixture and to complete the combustion. Figure 5 shows a cross section of a typical can; note that the geometry is more complex and curved

than the schematic of Figure 4. Note also that there is an internal structural wall surrounding the inner combustion area. The use of KIVA is often restricted to this inner area.



**Figure 3.** Schematics of the two common types of gas turbine combustors: (a) An annular combustor with a continuous region of combustion fed by several fuel injectors. (b) A set of combustion “cans” ringing the central shaft of the turbine.



**Figure 4.** Schematics of the general forms of a gas turbine combustor showing the two combustion zones, the exterior flow of air, and the various paths of air entering and within the combustion zone.

## 4 An Idealized, Simplified Combustor

It is apparent that one will have real difficulty in accurately approximating the flow in a combustor like that of Figure 5 with the geometry mechanisms of Figures 1 and 2. To discuss the nature of this difficulty, we introduce a simplified and idealized combustor, one that has cylindrical symmetry and less complicated geometry. This allows us to discuss the problem in 2D instead of 3D. The 2D cross-section of the idealized combustor is shown in Figure 6.

The flow in the combustor is modeled by domains (see Figure 2) which are composed of trapezoidal blocks (see Figure 1). Figure 7 shows three ways to decompose the shape of Figure 6 into domains. The boundaries of domains are shown by heavy dotted lines. The boundaries of the domains can also separate the three types of flow allowed in KIVA: (i) 2-phase flow with combustion, (ii) gas flow with combustion, (iii) flow without combustion.

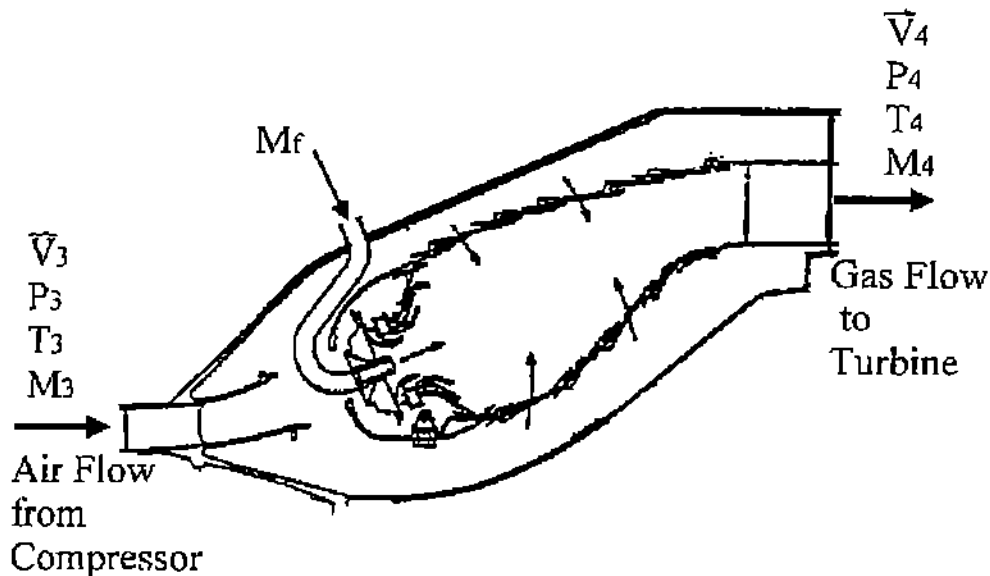


Figure 5. Cross section schematic of a gas turbine can with realistic (but rough) accuracy in the geometry of the can.

## 5 Geometry, Numerical, Code, and Modeling Problems

There are three potential types of difficulty in modeling the combustor shown in Figure 6 using KIVA as illustrated in Figure 7.

- *Geometry.* The flow boundaries must be linear so there are sharp corners at various points on the boundary. If only a few linear pieces are used then these corners introduce artificial disruptions into the flow. If the number of linear pieces is increased so that the combustor shape is well approximated and the flow is smooth, then a very fine KIVA grid must be used. At places where the combustor structural surface has real corners, one must use two or more KIVA domains in order to “break” the grid structure.
- *Numerical.* The grid structure is very tightly coupled in KIVA. The number of grid lines is constant in each direction within a domain even though the spacing can change. The number of grid lines between domains can change only in relation to the size of change in the boundary. This interdependence causes the finer grids needed at points of critical or complex flow (e.g., at the connections into the inner chamber, near the spray and flame fronts, where the flow meets structural obstacles) to propagate throughout the combustor. The exact nature of this propagation depends on the geometry but it is close to requiring a uniform grid in the entire combustor. The net result is that the entire combustor uses the finest grid (approximately) that is required at any part of the combustor. This, in turn, increases the time and memory used to compute the numerical solution. The examples in Figure 7 suggest that the proportion of “fine grid” is approximately doubled (from 1/3 to 2/3s) by the constraints on the grid structure. This, in turn, approximately doubles the number of grid lines required in each dimension which increases the number of volumes (and the computation) by a factor of at least 8. Using a continuously graded grid would probably reduce the computational effort by another factor of 2-4.
- *Code.* This discussion is only speculation pending a deeper look into the KIVA code. Even the simplified geometry requires that the domains in KIVA are connected in fairly complicated ways and that there be a substantial number (say 15 to 20) of them. KIVA might have been written with a simpler geometric model in mind and not allow so many domains or such complexity of interconnection. For example, if only 8 or 10 domains are used, there will be domains that contact three different structure boundaries and interface with three different flows. And this is only a 2D analysis; in 3D the number of domains, blocks and boundary/flow interfaces all increase.
- *Modeling.* This discussions is only speculation pending a closer look into the KIVA code. It appears that KIVA maintains physical reality (approximately) by satisfying the PDEs at every grid point (in every volume defined by the grid). Thus when two blocks or domains meet, the PDE is discretized on a grid that can be non-orthogonal. Such discretizations are, of course, easy (even if tedious) to derive and use. However, the accuracy of the discretization degrades from 2nd order to 1st order if this is done in a straightforward way. To maintain 2nd order accuracy requires much more complex discretization. If the non-orthogonality is small and the number of such points is small, the overall effect might also be small; then again, it might not be.

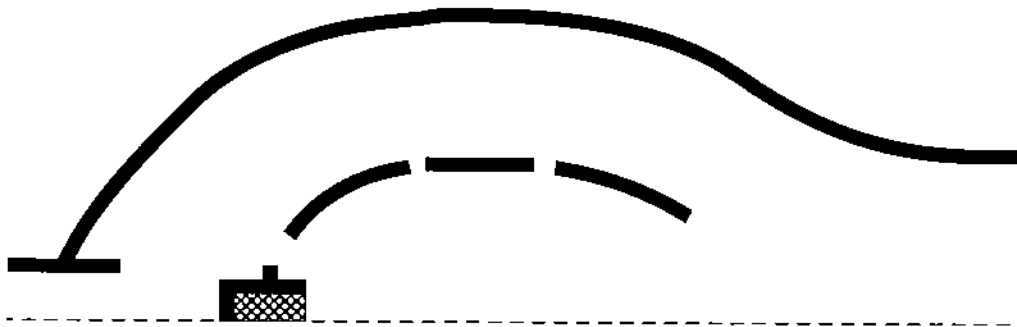


It appears that KIVA is designed to execute with predetermined boundary conditions, e.g., the inlet conditions are set by the preprocessor and then "inserted" into the main code. This does not imply these conditions are constant as they could be functions of time. However, it does imply that it will be awkward, if not infeasible, to connect KIVA to another code which is modeling the flow on the other side of the inlet boundary. Similarly, it may be difficult to run two separate KIVA models which interface with each other. At such an interface, the PDE is not satisfied so extra conditions must be enforced to maintain physical accuracy. The interface relaxation method, for example, can do this but if the preprocessor must be run each time the interface conditions change, this would probably be an unbearable overhead.

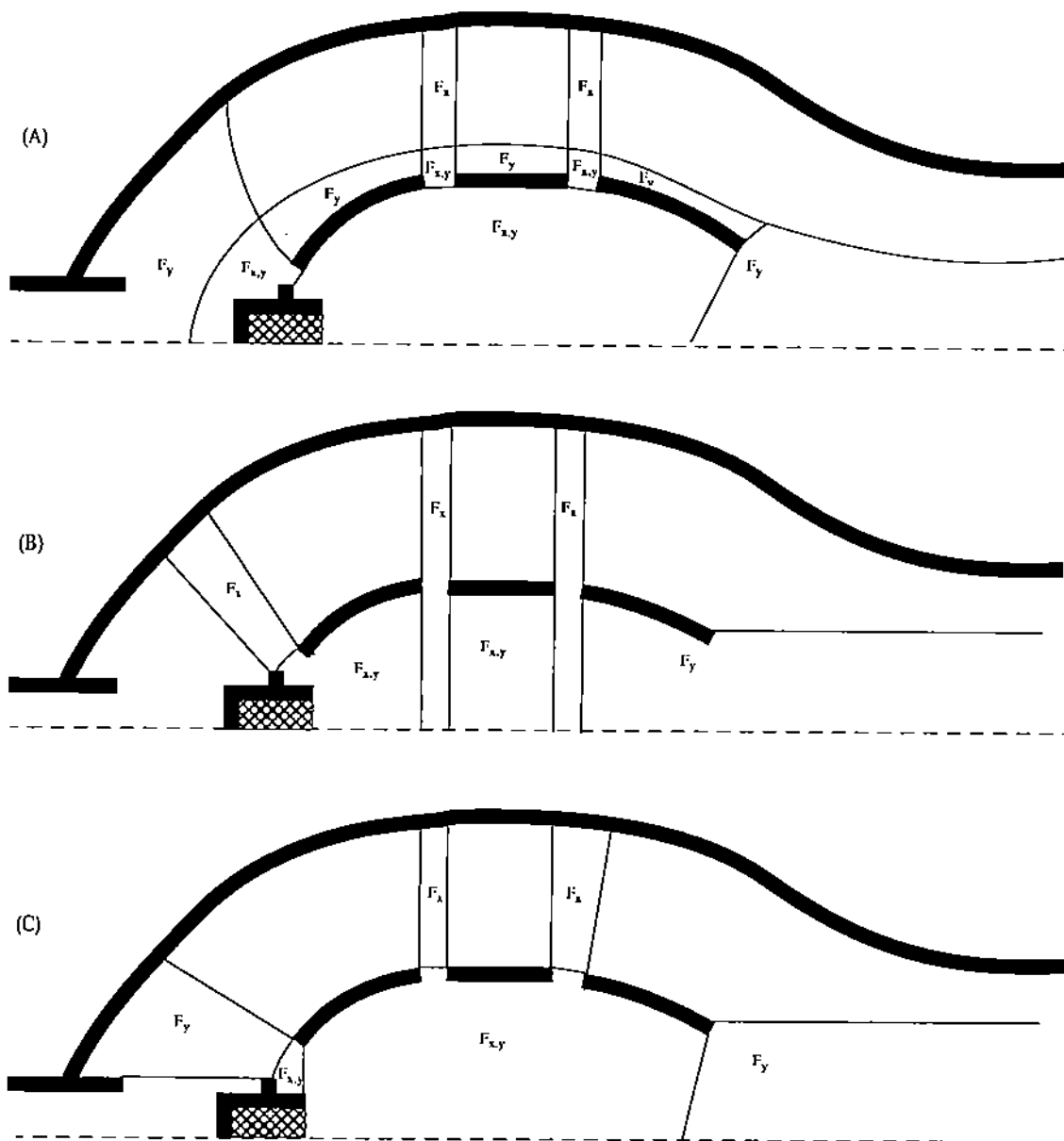
Most combustors have structural components "inside" the flow. These strongly affect the flow field itself so they cannot be neglected if high (even moderate) accuracy is desired. One should also consider if their physics should be modeled some. Two possible questions are: (i) Do their shapes change due to the high pressures and temperatures during operating? (ii) What are the temperature gradients across the structures and how much effect does the heat transferred have on combustor performance?

## 6 A Potential Remedy

In this section we discuss a remedy that might be feasible, i.e., that might exploit features already in KIVA or that might be accomplished with modest effort (compared to re-implementing KIVA). The principal problem that might be remedied is changing grid sizes. Interface relaxation can be used to connect two PDE solvers which use unrelated grids. We already have the tools for making this connection and must use them to connect KIVA to other solvers, e.g., ALE3D. So, once KIVA is put into this framework, one can change grid sizes between domains and thereby adjust this size somewhat to make the computation more efficient.



**Figure 6.** Cross section of an idealized, simplified gas turbine combustor which has rotational symmetry. The structural components (shaded) and fuel injection line (cross hatched) are shown thicker than reality so as to be seen easily. The lower half is the mirror image of the top half and is not shown here.



**Figure 7.** Three ways to insert KIVA domains into the shape of Figure 6. The domain boundaries are indicated by thin lines. Those domains with “fine” grids are labeled with  $F$ , the subscripts  $x, y$  or  $x, y$  indicate finess in the horizontal, vertical or both directions.

## References

1. A.A. Ameden, P.J. O'Rourke, and T.D. Butter, KIVA-II: A computer program for chemically reactive flows with sprays, Report LA-11560-MS, Los Alamos National Laboratory, May 1989, 158 pages.