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COMPARISON OF A SEMI-ANALYTIC AND A CFD MODEL OF URANIUM COMBUSTION TO EXPERIMENTAL DATA

By

Randy Clarksean
Clarksean and Associates
P. O. Box 51, New York Mills, MN 56567
Phone: 1 (218) 385-3750 Fax: 1(218) 385-3750
Email: clark@uslink.net

Charles W. Solbrig & Kenneth Bateman
Technology Development Division
Engineering Division
Argonne National Laboratory-West
P. O. Box 2528
Idaho Falls, ID 83403-2528

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Randy Clarksean
Clarksean and Associates
P.O. Box 51, New York Mills, MN 56567
Phone: 1.218.385.3750, Fax: 1.218.385.3751
Email: clark@uslink.net

Charles W. Solbrig and Kenneth Bateman
Argonne National Laboratory-West
P. O. Box 2528, Idaho Falls, ID 83403

ABSTRACT

Two numerical models were developed and compared for the analysis of uranium combustion and ignition in a furnace. Both a semi-analytical solution and a computational fluid dynamics (CFD) numerical solution were obtained. Prediction of uranium oxidation rates is important for fuel storage applications, fuel processing, and the development of spent fuel metal waste forms. The semi-analytical model was based on heat transfer correlations, a semi-analytical model of flow over a flat surface, and simple radiative heat transfer from the material surface. The CFD model numerically determined the flowfield over the object of interest, calculated the heat and mass transfer to the material of interest, and calculated the radiative heat exchange of the material with the furnace. The semi-analytical model is much less detailed than the CFD model, but yields reasonable results and assists in understanding the physical process. Short computation times allowed the analyst to study numerous scenarios. The CFD model had significantly longer run times, was found to have some physical limitations that were not easily modified, but was better able to yield details of the heat and mass transfer and flow field once code limitations were overcome.

INTRODUCTION

The tools available to an analyst have increased dramatically as the speed and use of the computer has increased. Prior to the wide development and sale of commercial heat transfer software, the analyst many times had to develop a unique model for each system being analyzed.

The model may have been as simple as a few node circuit analogy, or as complex as a several thousand line code for the solution of the Navier-Stokes equation.

Many institutions (universities, national laboratories, and industrial research and design centers) started to develop more general purpose software products in the late 1960's. The goal was to decrease the work of the analyst each time a new analysis had to be conducted. Many of these software products have evolved over time into very complex analysis packages. At present, there are numerous commercial software products on the market. The analyst still has to be knowledgeable of the physics of the problem he/she is trying to solve, plus be able to "tell" the software package how to solve the problem of interest.

The purpose of this work was to compare the time tested analytical solution method to a solution with one of the above mentioned computational fluid dynamics (CFD) codes. The semi-analytical model uses a heat transfer and a semi-analytical description of the flowfield and diffusion field for an idealized geometry. The CFD model used was FIDAP (FLUENT [9]). FIDAP is a commercially available general purpose finite element code used for the analysis of heat transfer and fluid mechanics.

The physical problem of interest is the oxidation of metals used in the nuclear industry. The present problem analyzes the reaction of uranium, but the techniques discussed here could be used for a wide range of metals. The real situations include the storage of spent nuclear fuel, fuel processing and handling operations, and the development of spent fuel metal waste forms.

At issue are metal fires. Metal fires can release large amounts of heat. When the metal is a nuclear fuel, or an intermediate waste product from the processing of nuclear fuel, it is important to be able to predict the reaction/heat release rates if the metal is inadvertently exposed to air. In certain configurations, such as a fine powder, the material can be pyrophoric at room temperature. The processing of spent fuel is planned at Argonne National Laboratory to develop metal waste forms. Operations of the facilities in which this processing will occur are impacted by the threat of a metal fire. The cell atmosphere is argon to prevent a fire from occurring but the safety analysis requires that an earthquake be analyzed where air is introduced into the processing cell. If a metal fire was to occur, heat would be released in the cell, cell pressure would increase, and if the pressure increased far enough, flow out of the cell could occur. The flow from the cell could result in the release of the gases to the environment. In order to prevent a release, sufficiently low levels of material are exposed within the cell to prevent the overpressure scenario presented here in case a worst case earthquake occurred. Calculating ignition temperature is not important since it is not an intrinsic property. However, the heat release is important because it drives the possible cell over pressure.

The remainder of the paper addresses the semi-analytical model, the CFD model, compares the results of both models with existing experimental data, and then discusses the advantages and disadvantages of each modeling approach.

SEMI-ANALYTICAL MODEL

The principal reaction of interest in the combustion of uranium is

$$U + O2 \rightarrow UO2 \qquad (1)$$

The isothermal oxidation rate of uranium has been measured by Baker [1] in oxygen at constant pressure (200 mm) from 300 to 625oC. The data were obtained in a metal "heat sink" reaction cell which minimized the temperature increase due to self-heating. High reaction rates prevented obtaining isothermal data above 625oC. A zeroeth order (that is, independent of concentration) Arrhenius reaction rate was fit to the initial slope of these data in Solbrig [2] as

$$dWO2/dt = 1.14x104 \text{ mg/cm2 min } \exp(-6946 \text{ K/T}) \qquad (2)$$

where WO2=oxygen deposited (mg/cm2), t = time (min), and T = temperature (K).

Baker provided the basis for the zero order reaction rate (that is, a rate independent of oxygen concentration) by comparing data in oxygen at different pressures [1] and in air [3].

Energy balance on the solid

To arrive at a heat balance on the solid in the manner of Baker [3], the following assumptions are made: 1) the temperature is spatially uniform in the solid, 2) the product of MmCp is invariant and is the same for the metal and the oxide, and 3) the reaction area does not change with time. The heat balance is:

$$M_m C_p \frac{dT}{dt} = \frac{Q}{10^3} \frac{M_U}{M_{02}} A \frac{dW_{02}}{dt} - hA(T - T_a) - \varepsilon\sigma A(T^4 - T_a^4) \qquad (3)$$

where Mm = mass of metal, Q = heat release per gram of Uranium reacted, A = surface area of metal, W02 = weight of oxygen added to fuel by reaction (mg/cm2), NOTE: 103 converts from g to mg, MU/MO2 = Molecular weight ratio of U to O2, (This ratio allows W02 to represent the weight of uranium reacted.) T = temperature of burning metal, assumed uniform throughout the metal and deposited oxide, and Ta = temperature of ambient gas in the furnace as well as the furnace temperature. Values used in this equation are as follows: CP = 0.044 cal/g K, Q=1089 cal/g U, Mu=238 g/mole, M02 = 32 g/mole, σ = 81.6 x 10-12 cal/cm2 min K4, ε = 0.75 and Ta starts at 300oC and increases at 10oC/min.

Heat transfer coefficients developed in Mouridian and Baker [4] are used here with the following gas phase properties: Cp=0.0883 Tf.165 (cal/gm K), k =1.062x10-4 Tf.65 (cal/min cm K), and ν =1.071x10-3 Tf1.605 (cm2/min) where Cp, k, and ν are the specific heat, thermal conductivity, and dynamic viscosity of the gas evaluated at the film temperature (average of T and Ta) and film concentration for air (90% nitrogen and 10% oxygen).

Forced convection heat transfer correlations were used for a horizontal cylinder Nu=0.38 (Re).5 where Nu = hL/k and Re = vL/v, the Nusselt number and Reynolds number, h = heat transfer coefficient, v is a representative velocity, and L is a representative length.

Baker [3] ran uranium combustion tests with cubes of metal in a furnace which were used to verify the model presented in this paper. The above correlations produced a representative Reynolds number of 200 for a test condition of v=500 cm/min oxygen (that is, 2500 cm/min air) and L=0.85 cm. This is laminar flow which is far below the turbulent flow transition criterion of roughly 2000. Thus, this justifies using laminar flow heat and mass transfer to model this system.

The emissivity of uranium varies with the amount of oxide on its surface. Baker [5] measured the emissivity of uranium for temperatures up to 1000oC. The emissivity is almost independent of phase and temperature but strongly dependent on oxide thickness. The value ranges from 0.31 for polished uranium to 0.76 for a deposition layer of 1 mg/cm2. Since the oxide layer builds up to 1 mg/cm2 very quickly, use of a constant 0.75 does not effect the results significantly.

Diffusion equation in the gas phase

The diffusion geometry is approximated by air flow over a flat plate of uranium where both sides are capable of reacting. The actual geometry of the reacting metal may be different from that of a flat plate, such as a cube, a wire, or a foil. The diffusion equation is written in the form

$$\frac{\partial X_{O_2}}{\partial t} + V_y \frac{\partial X_{O_2}}{\partial y} = D_{O_2} \frac{\partial^2 X_{O_2}}{\partial z^2} \qquad (4)$$

where XO2 is the molar concentration of O2, vy is the velocity of the gas parallel to the plate, DO2 is the diffusion coefficient of O2 relative to the gas mixture.

There are several assumptions implicit in this equation, some of which include, 1) the net molar flux normal to the plate, z direction, is zero, 2) the velocity in the z direction is zero, 3) the diffusion is small in the flow direction (y) compared to the convective term, and 4) the velocity profile in the y direction is known. The first and second assumptions are only partially true because there is a net molar flux of oxygen toward the plate where it is consumed and no gaseous product is produced to balance this out. An approximation to represent this flow (called Stephen flow) is presented in Mouridian [4] but is not used here. It increases the molar flux of oxygen to the surface because there is a pressure drop toward the surface. The third assumption is reasonable for sufficiently high flow rates. The y component of velocity assumption will be discussed later.

A further reasonable assumption is made that the transient term is small with respect to the convective term and is dropped from Equation 4. The boundary condition at y=0 is given as

$$XO2(t,0,z) = Xinlet(t) \qquad (5)$$

The inlet mole fraction, Xinlet, in the experimental data of Baker [3] is a constant. Even though the inlet mole fraction is a constant, the solution is a function of time because the reaction rate

boundary condition at the plate is time dependent. Since the time derivative is dropped from Eq. 4, no initial mole fraction can be specified. Two boundary conditions must be specified in the z direction. The boundary condition at $z = \delta$ is specified as being Xinlet. The boundary condition at $z = 0$ is a balance between the rate of oxygen diffusion and the reaction rate at the surface but is also limited by X02 = 0 is used to prevent negative concentration when the mass flux to the surface limits the reaction on the surface. See Reference 2.

Note that since the uranium temperature is assumed spatially uniform and since the reaction rate (that is, dWO2/dt) is independent of mole fraction, the reaction rate is the same for all values of y for a given time.

Reid [6] gives values for the diffusion coefficient of 0.181 cm2/sec for nitrogen-oxygen, 0.175 cm2/sec for air-oxygen at 273oC and 0.20 cm2/sec for argon-oxygen at 293oC. The value DO2 = 0.18 cm2/sec was used for all of the calculations presented here. These identical values were used for the CFD model.

Velocity Profile in the Gas Phase

The mass transport is highly dependent on the flow geometry. Flow over a cube can produce much more transport per unit area of exposed metal than can flow over a flat plate. The flow over a flat plate using the standard Blasius solution (constant properties) was used to represent the case of mass transfer off the surface of the cube. Other geometries were analyzed with the semi-analytical model, but will not be discussed here.

An approximate analytical solution for laminar flow over a flat plate was derived by Bird, Stewart, and Lightfoot [7]. The boundary layer thickness $\delta(y)$ with dynamic viscosity ν and velocity far from the plate V_∞, is

$$\delta(y) = 4.64\sqrt{\frac{\nu y}{V_\infty}} \qquad (6)$$

Note that $\delta(0) = 0$. The velocity profile is approximated as

$$\frac{V_y}{V_\infty} = \frac{3}{2}\left(\frac{y}{\delta(y)}\right) - \frac{1}{2}\left(\frac{y}{\delta(y)}\right)^3 ; 0 \le y \le \delta(y) \qquad (7)$$

Note that for air (ν=10.74 cm2/min and V_∞=500 cm/min) flowing over a 0.85 cm plate, the boundary layer at the end of the plate is $\delta = 0.135$ cm at 311 K.

Depending on the velocity and the length of the plate, the laminar boundary layer will break down into turbulent flow. Schlichting [8] states that the flow in the boundary layer remains laminar for Reynolds Number less than 5x105. The previously calculated Re of 40 for a cube of L=0.85 cm. indicates the flow will remain laminar for most cases of combustion of interest here. This velocity profile was used to represent flow over cubes by using the cube length. It will also

be used to model flow over a wire or sphere by taking a small value of L to represent its diameter. A finite difference technique was used for the solution of the diffusion and energy equations in the model.

CFD MODEL DEVELOPMENT

The second approach to modeling the uranium combustion process relied on a computational fluid dynamics (CFD) approach. The general-purpose finite element heat transfer and fluid dynamics code FIDAP (Fluent [9]) was used for this set of analyses. FIDAP can handle general three-dimensional geometries, for either transient or steady state problems.

The governing equations for the transient analyses of the reaction of the uranium in a heated gas stream included the Navier-Stokes (momentum) equations, the continuity equation, the energy equation, and a species transport equation.

$$\rho\frac{\partial\vec{u}}{\partial t}+\rho(\vec{u}\bullet\nabla)\vec{u}=-\nabla p+\mu\nabla^2\vec{u}+\rho\vec{g}\beta(T-T_o) \tag{8}$$

$$\nabla\bullet\vec{u}=0 \tag{9}$$

$$\rho C_p\frac{\partial T}{\partial t}+\rho C_p\vec{u}\bullet\nabla T=k\nabla^2T \tag{10}$$

$$\frac{\partial C}{\partial t}+\vec{u}\bullet\nabla C=D\nabla^2C \tag{11}$$

where $\vec{u}$, T, Cp, k, C, D, ρ, μ, β, are velocity, temperature, specific heat, thermal conductivity, species, concentration, diffusion coefficient, density, viscosity, and coefficient of thermal expansion. The axis-symmetric forms of the governing equations were solved. The actual geometry (described in the following section) was simplified from a cube in a tube to a cylinder in a tube. The three-dimensional nature of the problem would have been too time consuming to solve numerically. The surface area of the cylinder was set to be identical to that of the cube to best represent the surface reaction.

The boundary condition for the species transport equation and the surface reaction is:

$$-\rho\alpha_i\frac{\partial c_c}{\partial n}+c_iS=S_i \tag{12}$$

which is used in conjunction with the normal velocity condition.

$$\rho\vec{u}\cdot\vec{n}=S \tag{13}$$

where Si represents the surface reaction term and S is the sum of all reaction terms, including any reaction term for the gas stream. In the most general form S is defined as

$$S = \sum_{i=1}^{N} S_i, N = n_s + 1 \tag{14}$$

where ns represents the number species.

$$S_j = \sum_i \kappa_i (T)^{\beta_i} \exp\left(-\frac{E_i}{T}\right) \prod_k c_k^n \tag{15}$$

where

κi	=	reaction rate constant.
E	=	activation energy constant.
β	=	temperature power.
T	=	absolute temperature.
k	=	number of species reaction depends on.

For the present problem, the surface reaction was not assumed to depend on the species concentration nor temperature dependence in the coefficient term (temperature dependence does exist in the Arrhenius term). Making these simplifications reduces the surface reaction term to

$$S = \kappa \exp\left(-\frac{E}{T}\right) \tag{16}$$

where the constants are given in equation 2. The same surface reaction was used in both the semi-analytical and CFD models. No attempt was made to account for the buildup of oxide on the surface of the cube in the CFD model.

The boundary conditions for the momentum equation were no slip for the apparatus wall, parabolic inflow velocity profile, and a zero pressure gradient for the outflow boundary condition. The temperature boundary conditions were a function of time. To represent the heat-up of the apparatus, the inlet and wall temperatures were set at 10oC per min (same as used in experiments described next).

A schematic of the geometry modeled is shown in Figure 1 below. The finite element mesh used for the analyses is also shown in the figure. The finite element mesh shows the axis-symmetric characteristic of the geometry (r = 0 to r = router modeled).

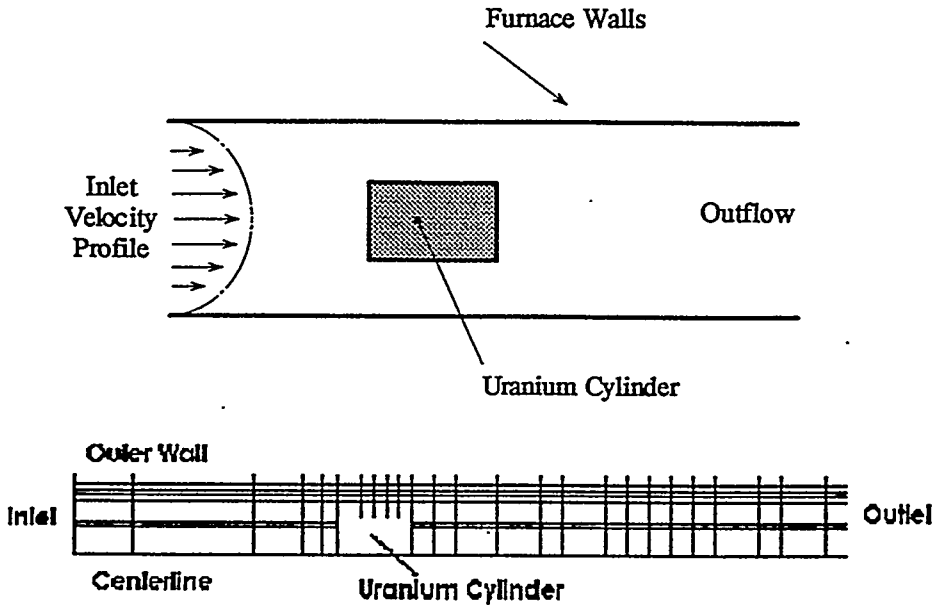

Figure 1 - General schematic of geometry (upper) and finite element mesh (bottom – mesh for cylinder not shown, 9 node quads) used for analyses.

During the use of FIDAP, it was discovered that the heat generated by the surface reaction was not coupled to the mass transfer to the surface of the cylinder. Both relationships were Arrhenius type relationships (see equations above). This results in the energy release on the surface only depending on the temperature of the surface – not the mass transfer to the surface. When mass transfer does not limit the reaction, the heat release is predicted correctly by the scheme presented above. But, once mass transfer to the surface determines the reaction rate on the surface, the heat release then depends on the rate of mass transfer – not just the temperature of the surface.

In order to overcome this limitation, a series of user subroutines were written to determine the mass transfer rate to the surface of the cube. The mass fluxes were then used to calculate the heat release rates on the surface of the uranium cylinder, rather than the Arrhenius rate equation. The determination of this limitation and the development of the user subroutines significantly increased the time required to analyze the problem.

COMPARISON OF NUMERICAL AND EXPERIMENTAL RESULTS

Baker [3] presented complete burning curves (i.e., a temperature time measurement through heatup, ignition, and combustion) of a 0.85 cm. cube of uranium. The experimental apparatus consisted of a reactor tube installed in a furnace. The reactor was a 2.54 cm diameter mullite tube clamped vertically in a combustion tube furnace. The cube had a small hole drilled in one face and was placed on top of a thermocouple suspended in the center of the tube. The oxidizing atmosphere entered the bottom of the reaction tube and flowed upward over the cube. It was preheated before reaching the sample by passage through ceramic beads packed in the lower

section of the tube. The furnace and oxidizing atmosphere were designed to be at the same temperature and both were increased at 10oC/min.

Fig. 2 presents results of Baker [3]. He was primarily interested in ignition temperature so he concentrated on reporting measurements in the low temperature regime but still reported some higher temperature results where most of the heat is released.

The velocity of air used was 2500 cm/min, which was five times that of the pure oxygen velocity. Results shown in Figure 2 are for both oxygen and air flow experiments. The two curves show similarity in the early part of the burning curves. The temperature in the oxygen experiment continued increasing until the thermocouple burned out. The specimen temperature in air increases to 1180oC at almost the same time as the specimen in oxygen but after a large increase, the temperature comes down to 800oC within five minutes. A second increase occurs within another five minutes, then another reduction to 1000oC before increasing a third time. The oscillations in the temperature are probably related to the buildup of oxide and the "flaking" off of the oxide during heating and reaction.

Results from the semi-analytical model are also presented in Fig. 2 for several free stream air velocities. An air velocity of 2500 cm/min (top line) can be directly compared with the experimental results. The semi-analytical curves show that the rapid temperature increase occurs about ten minutes before that of the experiment. After ignition, the temperature increases to 1050oC where it is limited by gas phase diffusion. Eventually, the temperatures in the analysis drop off when the metal is completely reacted..

The results from the CFD model are also shown in Fig. 2. The CFD analyses were conducted at different flow conditions and can be best compared with the semi-analytical results for a flow rate of 1250 cm/min, which are also included in Figure 2.

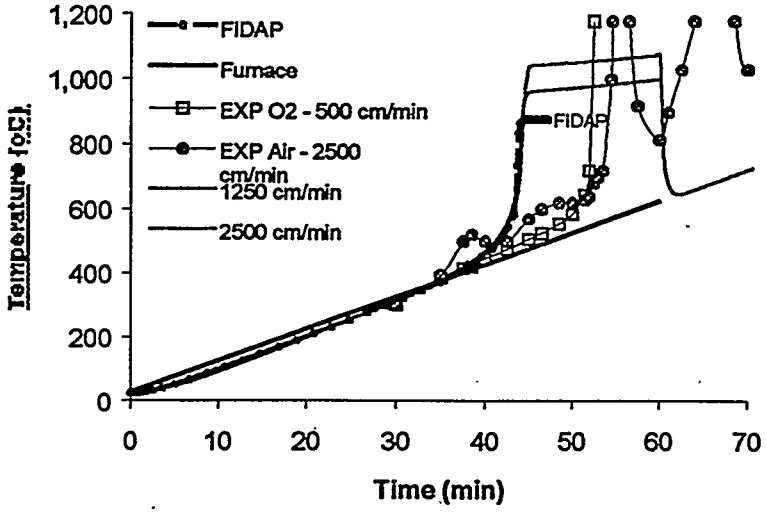

Figure 2 - Comparison of numerical and experimental results for the ignition of uranium in furnace. Temperature of the uranium cylinder versus time for uniform heating of the apparatus (10oC/min). FIDAP results are for surface node on the cylinder.

Both analyses (semi-analytical and FIDAP) compare well with the low temperature data (before "ignition"). A weakness of the semi-analytical model is the inability to calculate the distributed heat transfer rates because the cube is represented by flow over a flat plate instead of flow around a cube. The semi-analytical model relies on semi-analytical relationships for the flow field, and hence the mass transport. The CFD approach on the other hand eliminates the need for empirical relationships for the heat transfer and the semi-analytical flowfield. A weakness of the CFD approach is the long execution times needed to obtain this additional time for this highly non-linear problem.

The high temperature data (after "ignition") shows that both models do not describe the transient behavior in that region. The high temperature regime is diffusion controlled and is not dependent on the reaction rate. Changes to the mass transport modeling would significantly affect the transient heat release but improvements in the reaction rate model will not enhance the agreement. Instead, the improvement must come from better modeling the flow field, diffusion in the oxide and spalation of the oxide so the mass transfer is accurately modeled. Developing these models was not a goal of the work described here.

In general, there is good agreement between the semi-analytical and CFD model for the early portions of the ignition process. Once ignition occurs, there are significant differences between the two models. The point at which the reactions become mass limited are different. The roughly steady state temperatures for the mass diffusion limiting regions are approximately 100oC different, with the CFD model predicting a lower temperature.

The difference in the predicted temperature is due to the inability of the semi-analytical model to correctly predict the mass transfer to the cube. Figure 3 shows the flowfield over the uranium cylinder. The upstream portion of the cylinder has stagnation flow, which results in higher mass transfer rates. The flow behind the cylinder recirculates, which causes lower mass transfer in that region of the cylinder. Because the flowfield is assumed to be incompressible, the flow field is the same for all time steps.

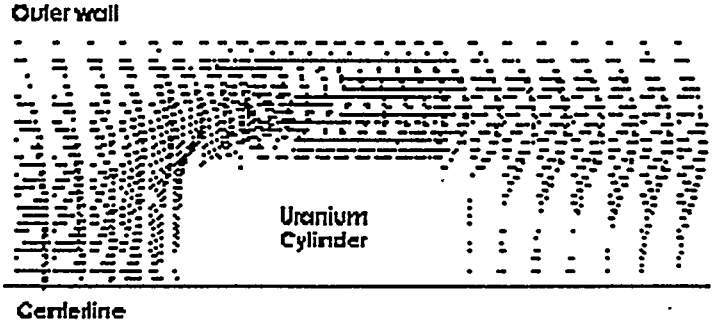

Figure 3 - Flowfield (velocity vectors) over and around uranium cylinder in the experimental apparatus. Viewed from the side of the cylindrical geometry used for the CFD analysis.

Figure 4 is a plot of the concentration profiles around the cylinder in the CFD model. The region behind the cylinder is highly depleted of oxygen once mass transfer limits the reaction on the

remainder of the cube. The fluid is depleted of oxygen as it flows past the cube. The fluid in the recirculation zone passes by the top of the cylinder (right hand side) at a much lower velocity and concentration, which reduces the heat generation by the upper cylinder surface.

COMPARISONS OF MODELING APPROACHES

The areas which were modeled in detail with the CFD model which were not modeled with the semi-analytic model were 1) conduction in the solid, 2) flow distribution around a cylinder, 3) heat transfer distribution around a cylinder, and 4) variations in the mass transfer around the cylinder.

Only small temperature gradients existed within the uranium cylinder (on the order of 1oC). This reinforced the validity of the spatially invariant temperature assumption used in the semi-analytical model. The details of the CFD model did demonstrate the effect of the flowfield on the temperature distribution within the cylinder. The temperatures of the upstream surface were higher than the downstream surface due to stagnation flow. The mass transfer around the cylinder also varies because of the flowfield. The semi-analytical model overpredicts the temperature of the cube once mass transfer limits the reaction because of the approximations made in analyzing the fluid flow, and hence the mass transfer. The semi-analytical model can not predict the recirculation zone nor its impact on the mass transfer.

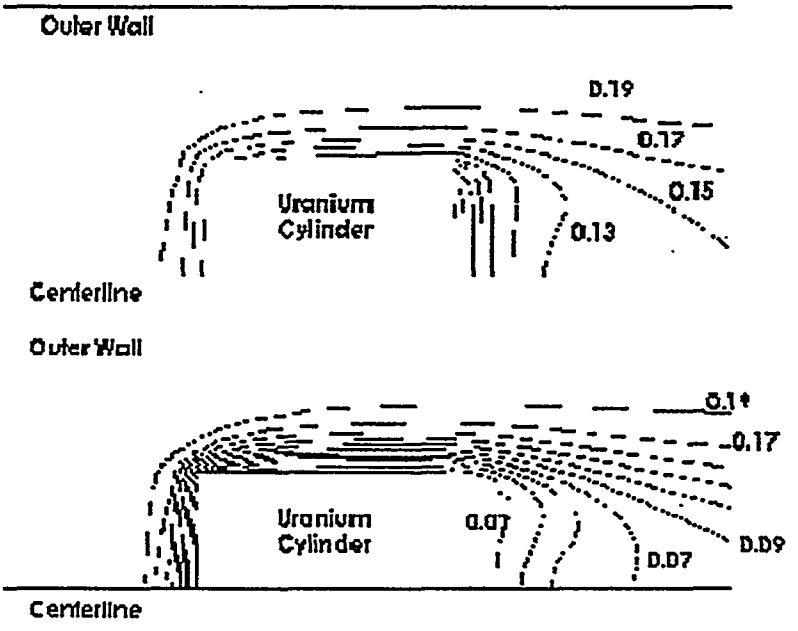

Figure 4 - Contour plot of species concentration prior to (upper) and after (lower) surface reaction is limited by mass transfer at the surface. Contours are equally spaced by 0.02% (max contour shown = 0.19). Upper contours are during the start of the ignition process, lower contours just after temperatures level off (mass diffusion limits reaction on surface).

Overall, both models did well in predicting the ignition of the uranium cylinder. Both models failed to predict temperature oscillations because physical models were not included in either

model to account for phenomenon that could have caused these oscillations. The semi-analytical model was quickly developed, required short computation times, and allowed the used to parametrically study the effects of different parameters on the solution. The semi-analytical model requires careful implementation for more complex geometries because it relies on empirical and estimated velocity profiles.

With the semi-analytical model, the equations can be studied to determine what terms in the model are important in the physical process. By studying these terms one can determine how the combustion process changes with parameters such as velocity, oxygen concentration, particle size, emissivity, etc. The CFD approach is more cumbersome for conducting parametric studies because of the large run times.

The semi-analytic model can be extended quickly and easily to other geometries as long as adequate empirical correlations exist. The semi-analytical approach may very well be the method of choice for future studies. However, the CFD approach would have to be used in cases where the accuracy of the heat release role in the diffusion-controlled regime is important. Using the CFD approach allows one to assess the assumptions made such as the effect of conduction in the solid and the impact of the flowfield on the heat and mass transfer. These affects can not be addressed in the semi-analytic model.

The CFD model required the development of user subroutines in order to overcome code limitations and took two orders of magnitude longer computing times (highly nonlinear nature of the governing equations and boundary conditions). The advantage of the CFD approach was the ability to analyze the changes in flow and mass transfer around the cylinder. This detailed information gave more realistic predictions of the cylinder temperatures and would be required for more complex geometries. The user of commercial CFD software has to be well aware of the proper physics of the problem when developing the detailed model. Without this knowledge, the user can solve the wrong problem, draw the wrong conclusions, and end up under or over designing the system of interest.

CONCLUSIONS

Realistic models of uranium combustion were developed here, which considered a heat balance on burning metal, the reaction rate of uranium oxygen, and the diffusion resistance of oxygen in an inert atmosphere to the metal surface. The models compare satisfactorily with experimental data for the prediction of the ignition of the uranium. Each of the modeling approaches had advantages and disadvantages. The semi-analytical model was quickly developed and allowed for rapid assessment of the impact of different variables on ignition. The CFD approach took more computational time, but better defined the flowfield and mass transfer to the cylinder. The semi-analytical model would be well suited for simple geometries (those with know empirical correlations) and the CFD model would be necessary to verify flowfield predictions when these are important to the mass transfer.

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