



## Modeling of Alkane Oxidation Using Constituents and Species

**This methodology is of interest to automobile manufacturers and other gas-turbine engine manufacturers.**

*NASA's Jet Propulsion Laboratory, Pasadena, California*

It is currently not possible to perform simulations of turbulent reactive flows due in particular to complex chemistry, which may contain thousands of reactions and hundreds of species. This complex chemistry results in additional differential equations, making the numerical solution of the equation set computationally prohibitive. Reducing the chemical kinetics mathematical description is one of several important goals in turbulent reactive flow modeling. A chemical kinetics reduction model is proposed for alkane oxidation in air that is based on a parallel methodology to that used in turbulence modeling in the context of the Large Eddy Simulation. The objective of kinetic modeling is to predict the heat release and temperature evolution. This kinetic mechanism is valid over a pressure range from atmospheric to 60 bar, temperatures from 600 K to 2,500 K, and equivalence ratios from 0.125 to 8. This range encompasses diesel, HCCI, and gas-turbine engines, including cold ignition.

A computationally efficient kinetic reduction has been proposed for alkanes that has been illustrated for n-heptane using the LLNL heptane mechanism. This model is consistent with turbulence modeling in that scales were first categorized into either those modeled or those computed as progress variables. Species were identified as being either light or heavy. The heavy species were decomposed into defined 13 constituents, and their total molar density was shown to evolve in a quasi-steady manner. The light species behave either in a quasi-steady or unsteady manner. The modeled scales are the total constituent molar density,  $N_c$ , and the molar density of the quasi-steady light species.

The progress variables are the total constituent molar density rate evolution and the molar densities of the unsteady light species. The unsteady equations for the light species contain contributions of the type gain/loss rates from the heavy species that are modeled consistent with the developed mathematical forms for the total constituent molar

density rate evolution; indeed, examination of these gain/loss rates shows that they also have a good quasi-steady behavior with a functional form resembling that of the constituent rate. This finding highlights the fact that the fitting technique provides a methodology that can be repeatedly used to obtain an accurate representation of full or skeletal kinetic models.

Assuming success with the modified reduced model, the advantage of the modeling approach is clear. Because this model is based on the  $N_c$  rate rather than on that of individual heavy species, even if the number of species increases with increased carbon number in the alkane group, providing that the quasi-steady rate aspect persists, then extension of this model to higher alkanes should be conceptually straightforward, although it remains to be seen if the functional fits would remain valid or would require reconstruction.

*This work was done by Josette Bellan and Kenneth G. Harstad of Caltech for NASA's Jet Propulsion Laboratory. For more information, contact [iaoffice@jpl.nasa.gov](mailto:iaoffice@jpl.nasa.gov). NPO-46792*

## Fabrication of Lanthanum Telluride 14-1-11 Zintl High-Temperature Thermoelectric Couple

**This methodology will aid device fabrication for waste energy recovery applications in cars, power plants, and industrial processes and machinery.**

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The development of more efficient thermoelectric couple technology capable of operating with high-grade heat sources up to 1,275 K is key to improving the performance of radioisotope thermoelectric generators. Lanthanum telluride  $\text{La}_{3-x}\text{Te}_4$  and 14-1-11 Zintl ( $\text{Yb}_{14}\text{MnSb}_{11}$ ) have been identified as very promising materials.

The fabrication of advanced high-temperature thermoelectric couples requires the joining of several dissimilar materials, typically including a number of diffusion

bonding and brazing steps, to achieve a device capable of operating at elevated temperatures across a large temperature differential (up to 900 K). A thermoelectric couple typically comprises a heat collector/exchanger, metallic interconnects on both hot and cold sides, n-type and p-type conductivity thermoelectric elements, and cold-side hardware to connect to the cold-side heat rejection and provide electrical connections.

Differences in the physical, mechanical, and chemical properties of the materials

that make up the thermoelectric couple, especially differences in the coefficients of thermal expansion (CTE), result in undesirable interfacial stresses that can lead to mechanical failure of the device. The problem is further complicated by the fact that the thermoelectric materials under consideration have large CTE values, are brittle, and cracks can propagate through them with minimal resistance.

The inherent challenge of bonding brittle, high-thermal-expansion thermoelectric materials to a hot shoe material



The High-Temperature Couple made of  $\text{La}_{3-x}\text{Te}_4$  and  $\text{Yb}_{14}\text{MnSb}_{11}$ .

that is thick enough to carry the requisite electrical current was overcome. A critical advantage over prior art is that this device was constructed using all diffusion bonds and a minimum number of assembly steps.

The fabrication process and the materials used are described in the following steps:

(1) Applying a thin refractory metal foil to both sides of lanthanum tel-

luride. To fabricate the n-type leg of the advanced thermoelectric couple, the pre-synthesized lanthanum telluride coupon was diffusion bonded to the metal foil using a thin adhesion layer.

- (2) Repeating a similar process for the 14-1-11 Zintl p-type leg of the advanced thermoelectric couple.
- (3) Bonding thick CTE-matched metal plates on the metallized lanthanum

telluride and  $\text{Yb}_{14}\text{MnSb}_{11}$  to form the hot and cold sides of the thermoelectric couple.

The calculated conversion efficiency of such an advanced couple would be about 10.5 percent, about 35 percent better than heritage radioisotope thermoelectric technology that relies on Si-Ge alloys. In addition, unlike Si-Ge alloys, these materials can be combined with many other thermoelectric materials optimized for operation at lower temperatures to achieve conversion efficiency in excess of 15 percent (a factor of 2 increase over heritage technology).

*This work was done by Vilupanur A. Ravi, Billy Chun-Yip Li, and Jean-Pierre Fleurial of Caltech and Kurt Star of UCLA for NASA's Jet Propulsion Laboratory. Further information is contained in a TSP (see page 1).*

*In accordance with Public Law 96-517, the contractor has elected to retain title to this invention. Inquiries concerning rights for its commercial use should be addressed to:*

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## A Computer Model for Analyzing Volatile Removal Assembly

*John H. Glenn Research Center, Cleveland, Ohio*

A computer model simulates reactional gas/liquid two-phase flow processes in porous media. A typical process is the oxygen/wastewater flow in the Volatile Removal Assembly (VRA) in the Closed Environment Life Support System (CELSS) installed in the International Space Station (ISS). The volatile organics in the wastewater are combusted by oxygen gas to form clean water and carbon dioxide, which is solved in the water phase. The model

predicts the oxygen gas concentration profile in the reactor, which is an indicator of reactor performance.

In this innovation, a mathematical model is included in the computer model for calculating the mass transfer from the gas phase to the liquid phase. The amount of mass transfer depends on several factors, including gas-phase concentration, distribution, and reaction rate. For a given reactor dimension, these factors depend on pressure and

temperature in the reactor and composition and flow rate of the influent.

*This work was done by Boyun Guo of the University of Louisiana at Lafayette for Glenn Research Center. Further information is contained in a TSP (see page 1).*

*Inquiries concerning rights for the commercial use of this invention should be addressed to NASA Glenn Research Center, Innovative Partnerships Office, Attn: Steve Fedor, Mail Stop 4-8, 21000 Brookpark Road, Cleveland, Ohio 44135. Refer to LEW-18369-1.*