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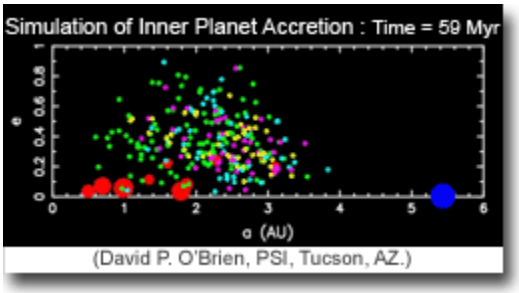


(David P. O'Brien, PSI, Tucson, AZ.)

Dynamics and Chemistry of Planet Construction

--- Planetary compositions allow us to test computer models of planet formation.

Written by G. Jeffrey Taylor
Hawai'i Institute of Geophysics and Planetology

Sophisticated calculations of how planetesimals assembled into the terrestrial planets can be tested by using models of the chemistry of the solar nebula. Jade Bond (previously at University of Arizona and now at the Planetary Science Institute, Tucson, AZ), Dante Lauretta (University of Arizona) and Dave O'Brien (Planetary Sciences Institute) combined planetary accretion simulations done by O'Brien, Alessandro Morbidelli (Observatoire de Nice, France), and Hal Levison (Southwest Research Institute, Boulder) with calculations of the solar nebula chemistry as a function of time and distance from the Sun to determine the overall chemical composition of the planets formed in the simulations. They then compared the simulated planets with the compositions of Earth and Mars. The simulated planets have chemical compositions similar to real planets, indicating that the accretion calculations are reasonable. Questions remain about the accretion of water and other highly volatile compounds, including C and N, which are essential for life.

References:

- Bond, J. C., Lauretta, D. S., and O'Brien, D. P. (2010) Making the Earth: Combining Dynamics and Chemistry in the Solar System. *Icarus,* v. 205, p. 321-337. doi:10.1016/j.icarus.2009.07.037
- O'Brien, D. P., Morbidelli, A., and Levison, H. F. (2006) Terrestrial Planet Formation with Strong Dynamical Friction. *Icarus,* v. 184, p. 39-58. doi:10.1016/j.icarus.2009.04.005

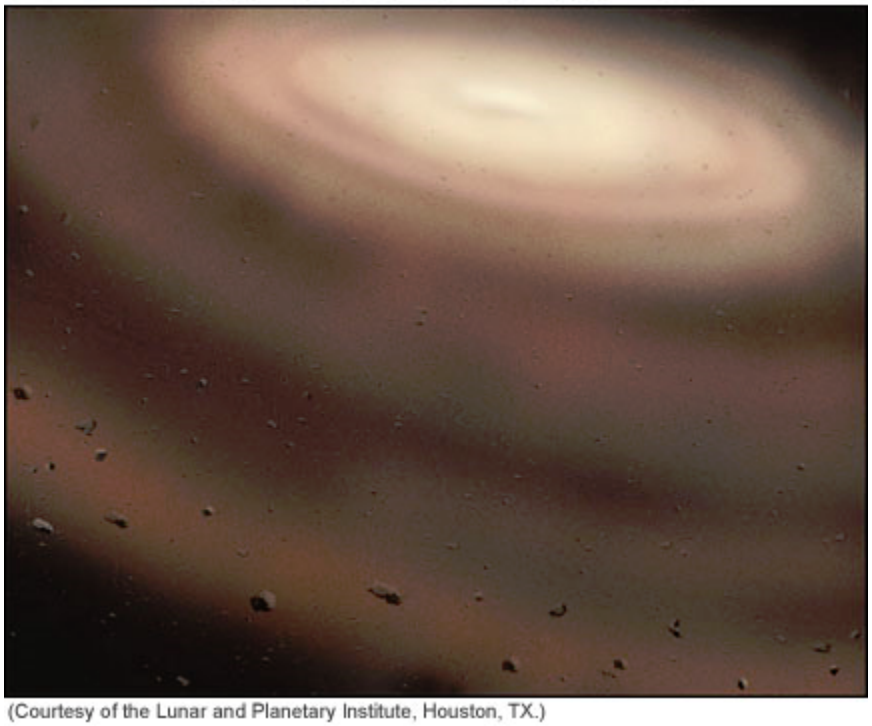
PSRDpresents: Dynamics and Chemistry of Planet Construction --Short Slide Summary (with accompanying notes).

Making Planets

Both theory and astronomical observations of young stars indicate that when the Sun formed it was surrounded by a disk of dust and gas. According to physicists who study the dynamics of the disk that must have orbited the Sun, planet formation began when dust grains clumped together and grew, forming objects up to a few kilometers across. Those hefty rocks rapidly accreted (possibly taking only a hundred thousand years) to form planetary embryos, which were roughly Moon to Mars-sized bodies. The planetary embryos took a more leisurely tens of millions of years to whack into each other and to gather up left over smaller objects to form the inner planets.

The step from small planetesimals to planetary embryos was fairly orderly, with each embryo forming in its own relatively narrow feeding zone. Their compositions, therefore, reflected the composition of the dust in that region of the solar disk, and two embryos growing near each other would have had similar compositions. The accretion of planetary embryos into terrestrial planets was much more disorderly. Planetary embryos interacted with each other and with the large outer planets, causing changes to their orbits. The result was that when they collided, they did not necessarily come from the same neighborhood of the solar disk. This process has been modeled quantitatively by many investigators.

Artist's Rendition of Planetesimals



(Courtesy of the Lunar and Planetary Institute, Houston, TX.)

Within the solar nebula, dust and ice particles embedded in the gas moved, occasionally colliding and merging, growing into larger bodies, called planetesimals, a few kilometers across. Close to the Sun, within the about 1.5 AU (the orbit of Mars), planetesimals were composed mostly of silicates and metallic iron. Further away from the juvenile Sun where it was colder, water ice and other volatile compounds were much more abundant. Delivery of water to the inner planets during accretion requires mixing planetesimals from a range of distances from the Sun. Jade Bond and her colleagues studied the bulk chemical compositions of planets formed in computer simulations of accretion, concluding that the simulations reproduce planet compositions reasonably well. Image provided courtesy of the Lunar and Planetary Institute.

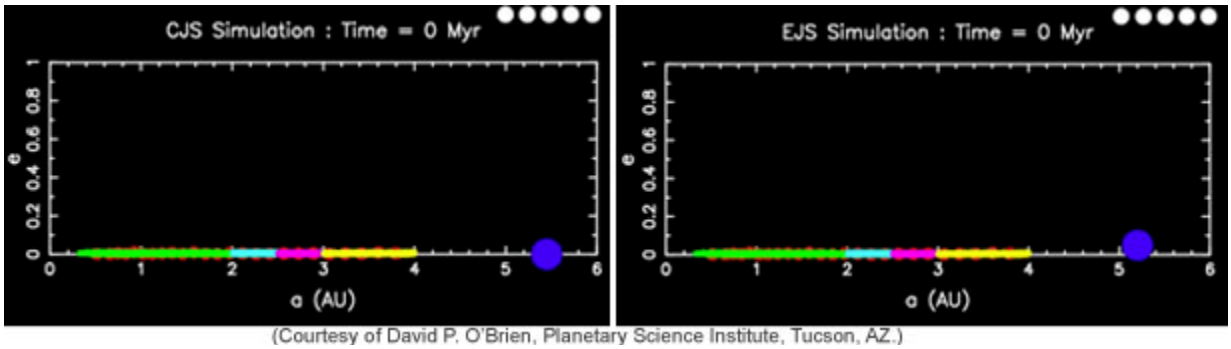
The simulations use classical equations of motion to follow planetesimal orbits and their gravitational effects on each other. The equations are solved by numerical techniques using computers that allow investigators to follow numerous bodies as their positions in space vary. To implement the calculations, O'Brien and his coworkers use an efficient algorithm written by Hal Levison and colleagues called the symplectic massive body algorithm, or SyMBA for short. The trick in developing an appropriate algorithm is that it accurately reflects the underlying equations that describe the physics and uses a minimum amount of computer time.

In all the simulations, the growing planets become smaller in number and bigger in size as the calculations grind away inside a computer. Most important, the embryos migrate inwards and outwards due to gravitaitonal perturbations before before accreting with one another. This causes considerable shuffling throughout the inner solar system and even two planets that grow in the same region can end up with different compositions. The simulations generally form about the right number of inner planets, but two problems surface. First, the final planetary orbits have higher eccentricities (deviation from perfectly circular orbits)

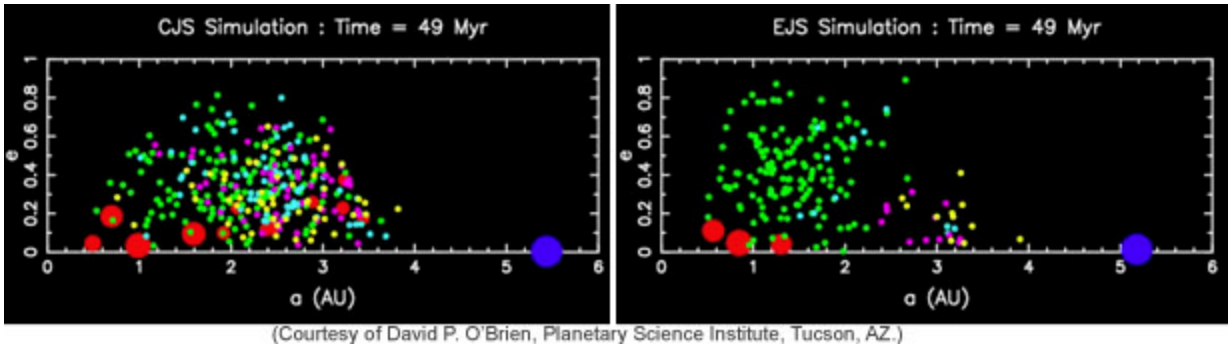
and inclinations (above or below the mid-plane of the accretion disk surrounding the Sun). Second, formation of the simulated planets also takes longer than cosmochemists have determined from age dating of rocks from the Earth, Moon, and Mars.

Planetary dynamicists knew that overcoming these problems would require including more planetesimals in the simulations. They reasoned that more planetesimals interacting with planetary embryos would cause more rapid accretion and less elliptical and inclined orbits. The underlying cause is that the smaller bodies (planetesimals) acquire higher velocities, but the larger bodies (embryos) remain slower. Dynamicists call this process "dynamical friction." Thus, the relative velocities of planetary embryos remain low, enhancing the chance that they accrete to each other. The problem is that adding more planetesimals results in more demands on the computers doing the calculations. Earlier calculations used 100 to 200 planetesimals. O'Brien and colleagues used about 1000. (Advances in computer capabilities come rapidly. In their 2006 paper, O'Brien and colleagues cite previous studies published between 2002 and 2004, and write, "...the simulations were limited to 100-200 bodies by the computers of the time..." Of *the time*? That time was only a *few* years before. Clearly, time is not linear in the world of computers!)

O'Brien's simulations produce about the right number of inner planets (3 or 4), with appropriate orbital parameters and accretion times of 30 to 70 million years, consistent with cosmochemical data. He and his colleagues did two sets of simulations. One begins (nicknamed CJS) with Jupiter and Saturn in circular orbits in the same plane, as predicted by the "Nice model," named for Nice, France, where co-author Morbidelli works and other dynamacists have spent considerable time. The other (EJS) begins with Jupiter and Saturn in their present elliptical orbits. The EJS simulations result in considerably less mixing throughout the inner Solar System than do the CJS simulations, a potentially testable difference. In particular, the EJS simulations do not cause delivery of water-bearing planetesimals from the outer asteroid belt (more than 2.5 astronomical units from the Sun), whereas the CJS result in wetter inner planets. You can watch the simulation movies online; frames at Time=0 and Time=49 Myr are shown below. X-axis is semimajor axis (AU) and y-axis is eccentricity.

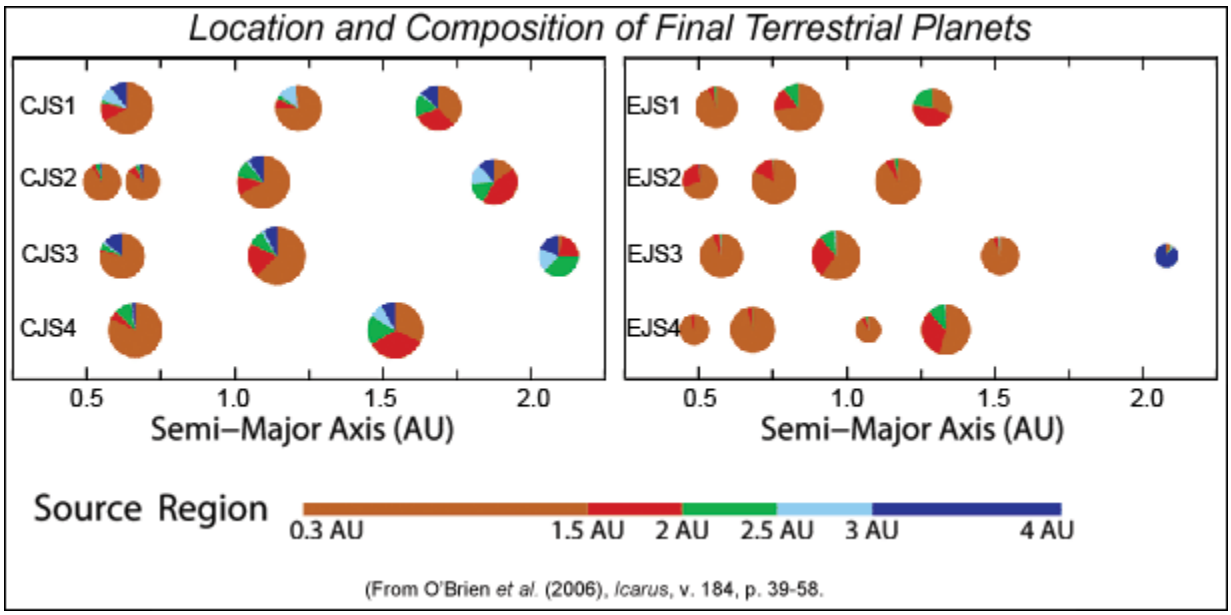


(Courtesy of David P. O'Brien, Planetary Science Institute, Tucson, AZ.)



(Courtesy of David P. O'Brien, Planetary Science Institute, Tucson, AZ.)

Two simulations of accretion of the inner planets. Both simulations begin with half the mass in large bodies with masses equal to about 10% of Earth's present mass (about the size of Mars), and half is in bodies that are 1/40 as massive as the embryos. In the simulation on the left (CJS), Jupiter and Saturn begin in circular orbits. In the one on the right (EJS), Jupiter and Saturn begin in their less-circular present orbits. Time=0 Myr is on top. Time=49 Myr is on the bottom. Note the much more significant mixing of planetesimals (sideways motions) in the CJS simulation than in the EJS simulation.



These pie diagrams show the results of all of Dave O'Brien's simulations for Jupiter and Saturn in circular orbits (CJS) and in their present elliptical orbits (EJS). The pie diagrams are proportional to planet sizes and show the contributions of material from different distances from the Sun, in astronomical units (AU). The CJS simulations result in planets that receive contributions from a much wider range of locations than do the EJS simulations. This has implications for the final compositions of the planets, a motivation for the work done by Jade Bond. (The chemical simulations actually used a much finer radial resolution to determine the abundances than just the five regions shown in these pie diagrams.)

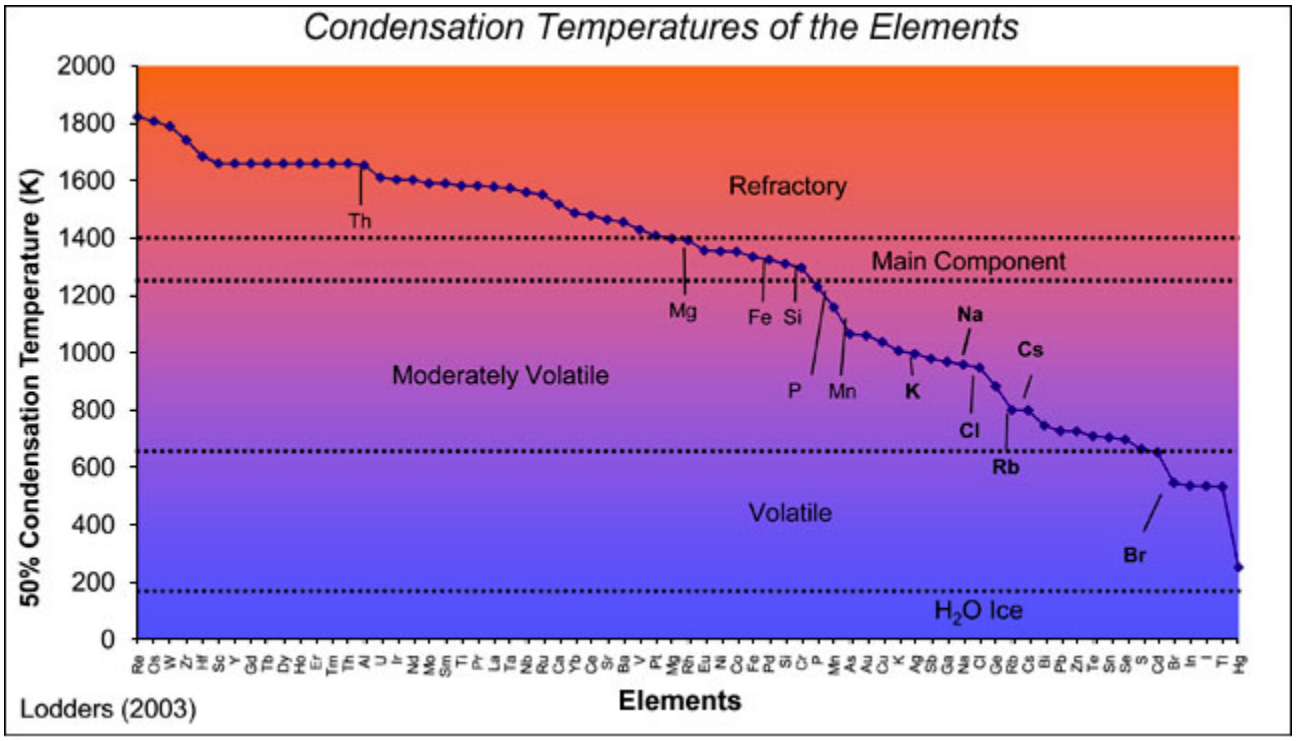
These elaborate simulations of planet formation are impressive, but lack independent tests of their veracity. Comparison of the bulk chemical composition of the simulated planets to the bulk chemical compositions of Earth and Mars could be a useful test. That is what Jade Bond and her coworkers set out to do.

Using Nebular Chemistry

The cloudy disk of gas and dust surrounding the gestating Sun contained different solids and gases depending on the temperature, which varied with location and time. In general, it was hotter closer to the Sun than farther from it, but also cooled from whatever maximum was reached at any specific distance from the Sun. Cosmochemists have a long tradition of trying to determine what solids and gases were in equilibrium with each other as a function of temperature in the disk (also called the solar nebula). The calculations are complicated. They use hundreds of different gas, mineral, and liquid compounds and associated thermodynamic data to determine what solids, liquids, and gases are in equilibrium at a given temperature. The calculations almost always assume equilibrium, greatly simplifying the arduous calculations (which are done on a computer). On top of that, the results vary depending on the ratio of dust to gas. A good example of the effect of the dust/gas ratio is given by Denton Ebel (American Museum of Natural History, New York). [See http://research.amnh.org/~debel/vapors1/vapors1.html. Link opens in a new window.]

Assuming equilibrium and a disk composition like that of the most primitive carbonaceous chondrites, the elements condense over a wide range of temperatures, as shown in the graph below. All the abundant elements such as magnesium (Mg), iron (Fe), and silicon (Si) begin to condense above 1200 Kelvin. They are, therefore, always in solids below that temperature. Others condense to solids at lower temperatures--around 900 to 1000 Kelvin for the alkali elements potassium (K), rubidium (Rb) and cesium (Cs), and still others condense below 600 Kelvin. Water does not condense as ice until about 180 Kelvin, accompanied at somewhat lower temperature by nitrogen and carbon compounds. Thus, the essentials for life--water, carbon, and nitrogen--only enter solid phases at quite low temperature, less than 180 Kelvin (-93 Celsius). Such

temperatures apply to the region of the solar nebula substantially beyond the present orbit of Mars.



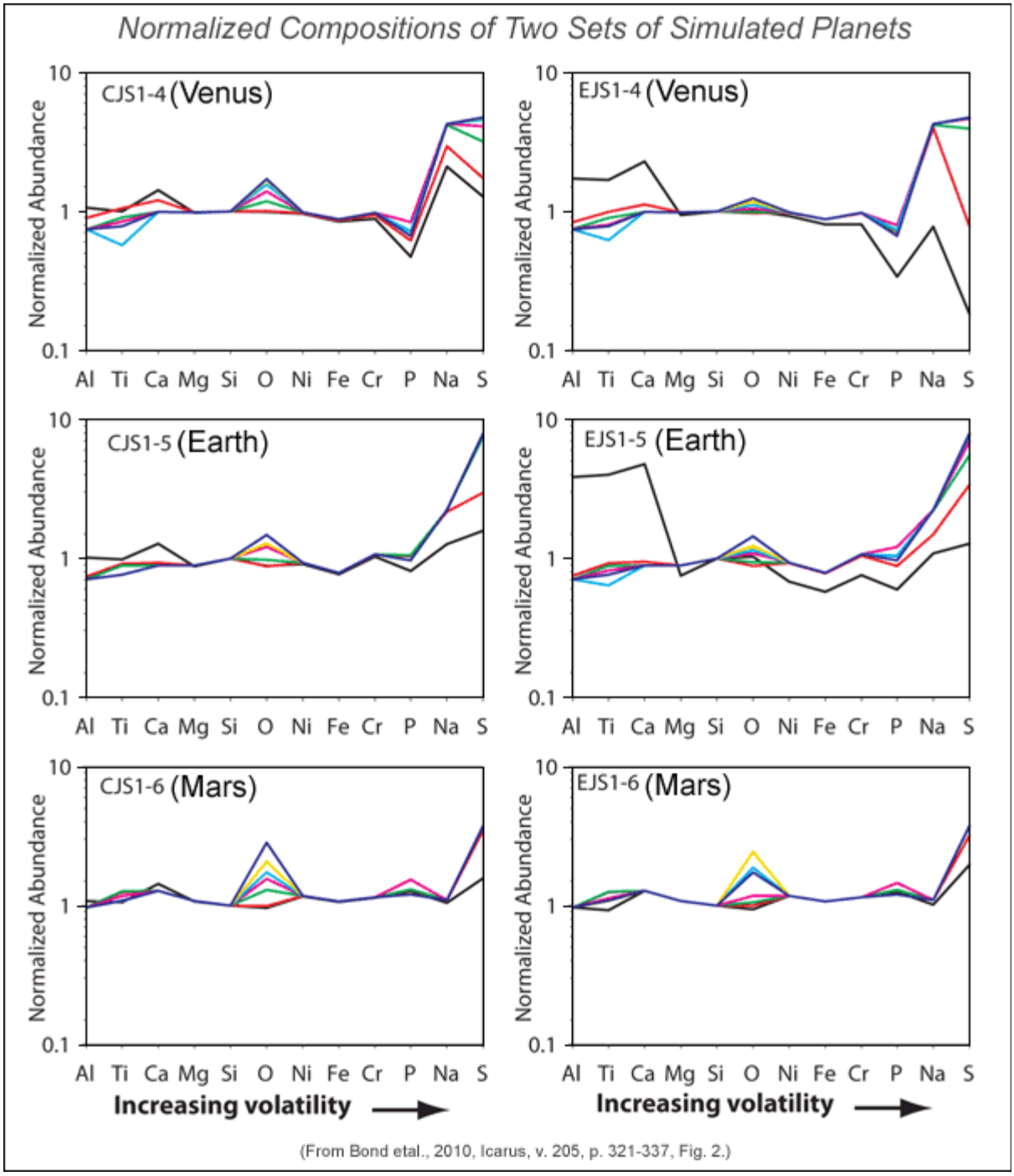
(PSRD graphic based on calculations done by Katarina Lodders, Washington University in St. Louis.)

Temperature (Kelvin) at which 50% of an element is condensed to a solid, calculated using the abundances of the elements in the Solar System, thermodynamic data, and numerous equations that must be solved simultaneously. The horizontal axis simply lists the elements in order of decreasing condensation temperature. High-temperature elements are called refractory; those with lowest condensation temperatures are called volatile elements.

Combined Chemistry and Dynamical Modeling

Cosmochemists and astrophysicists have modeled the temperature and pressure variations and cooling time of the solar nebula. Combining these estimates with the condensation sequence allowed Jade Bond to estimate the composition of the solids at different temperatures and distances from the Sun. Merging this with the results of O'Brien's simulations (see pie diagrams above) at different times during the cooling of the solar nebula, Bond and coworkers were able to estimate the compositions of the planets produced by all the simulations.

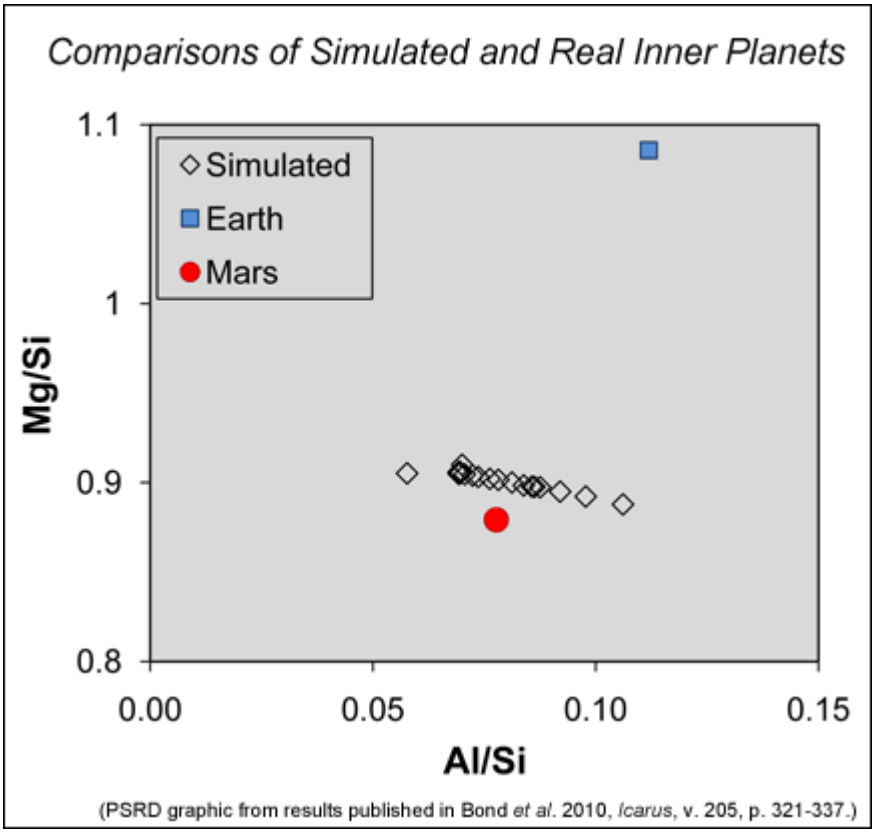
One interesting result is that the simulated planets have compositions that depend on the formation times of the planetesimals composing them. As shown by the different-colored lines in the diagrams below, as time increases from 0.25 million years to 3 million years, the concentrations of the volatile elements (Na and S) increase. This happens because the nebula is hotter during earliest times, so volatile elements are not condensed except far from the Sun. As the nebula cools, volatile elements condense closer to the Sun. The diagrams show "normalized compositions," a parameter often used in cosmochemistry. In this case the inferred composition of each simulated planet is divided by the bulk composition of Earth or Mars, depending on its location. Both the simulated and real planet compositions are also divided by their silicon contents. This allows for easy comparison because a simulated planet identical to its real counterpart would plot as a horizontal line at 1 in the figure below.



Normalized compositions of two sets of simulated planets run under the assumptions of circular (CJS) or elliptical (EJS) orbits for Jupiter and Saturn. Perfect agreement would be shown as a horizontal line at 1. The colored lines represent times during cooling of the solar nebula (black: 250,000 years; red: 500,000 years; green: 1,000,000 years; pink: 1,500,000 years; light blue: 2,000,000 years; yellow: 2,500,000 years; and dark blue: 3,000,000 years). Note that volatile elements (Na and S) increase in abundance with increasing time and tend to be higher in the simulated planets than the real ones. Jade Bond and her coworkers suggest that the best fit to the real planets is the red line, corresponding to 500,000 years.

The simulated planets do not differ drastically from the compositions of Earth and Mars, as determined from analyses of rocks and surface materials in them. For example, the diagram below shows the magnesium/silicon and aluminum/silicon ratios of simulated planets (both CJS and EJS cases) formed 500,000 years after the start of accretion. (Simulated planets formed at later times have the same relative abundances of the three elements plotted in the diagram below.) The match to the simulated planets is good for Mars, but Mg/Si is notably low compared to Earth. Bond and her colleagues discuss possible reasons for this

discrepancy. One is that the Earth was made mostly from materials closer to the Sun (0.1 to 0.7 AU) than the models indicate, suggesting much more radial mixing than the shown in the simulations. They consider this unlikely because not enough material was located in that region of the solar nebula to form the Earth. Another possibility is that the solids formed at high temperature (hence high in magnesium) accrete into bodies before the temperature falls significantly, leading to lower silicon and higher magnesium/silicon ratios. Other possibilities include how much silicon is sequestered into the metallic cores of the different planets, and varying ratios of dust to gas in the nebula, perhaps driven by turbulence (see **PSRD** article Tiny Molten Droplets, Dusty Clouds, and Planet Formation).



Compositions of Earth, Mars, and simulated inner planets are represented on this plot of the magnesium/silicon ratio to the aluminum/silicon ratio. The simulations do not match the composition of Earth, but do match well for Mars.

Water and Other Volatiles

This issue of how Earth and the other terrestrial planets acquired their water is of central importance to understanding planetary accretion, the processes operating when planets initially melted, and the origin of life. Cosmochemists have proposed several mechanisms: Delivery during accretion of planetesimals formed at more than 2.5 AU from the Sun, chemical reactions with nebula gases to form hydrous minerals, adsorption of water onto dust grains before they accreted to form planetesimals, and later delivery by comets.

Dave O'Brien's simulations explore only the case of accretional processes transporting cooler, water-bearing planetesimals from the outer asteroid belt to the inner terrestrial planet region. In the simulations where Jupiter and Saturn are in elliptical orbits initially, far less water is delivered to the terrestrial planets than in the case where the giant planets are in initially circular orbits. However, as Jade Bond and her coworkers point out it is possible that adsorbed water was incorporated into the planetesimals that form the basis of their simulations. Michael Drake (University of Arizona) and his coworkers have argued that the solids, when still dust grains, would have been bathed in a vapor rich in H_2O. These dust grains would accrete into

planetesimals, becoming passengers in objects involved in planet formation. Thus, delivery of at least some of the water may be a natural consequence of planet formation.

But are water and other volatiles preserved as the planets grow? The larger the planets become, the more energetic the accretionary impacts are. Jade Bond considers loss of volatiles by impact, showing that the discrepancies between the volatile contents of the simulated planets and those of the real ones can be alleviated by loss caused by impacts as the planets grew. This is a topic that needs to be examined in more detail.

Planet Compositions: We Need to Know More

Understanding how planets formed is one of those fundamental questions in cosmochemistry. Progress is clearly being made, but the whole story described above is a bit of a house of cards. We model planetary accretion, model the temperature history of the solar nebula, and model the composition of the nebula at different temperatures and pressures. From all that we estimate the compositions of the planets formed in the simulations and compare them to the actual planets in the inner Solar System. The comparison with real planets certainly seems like a good test of all that modeling, but aspects of our assessment of the compositions of the real Earth and Mars are not known well and depend on (you guessed it) modeling, or at least some assumptions. Nevertheless, cosmochemists are making progress on all fronts and Jade Bond's integrated study combining accretion, solar nebula chemistry, and planet compositions points the way forward.

Additional Resources

LINKS OPEN IN A NEW WINDOW.

- **PSRDpresents:** Dynamics and Chemistry of Planet Construction --Short Slide Summary (with accompanying notes).

- Bond, J. C., Lauretta, D. S., and O'Brien, D. P. (2010) Making the Earth: Combining Dynamics and Chemistry in the Solar System. *Icarus,* v. 205, p. 321-337. doi:10.1016/j.icarus.2009.07.037
- Drake, M. J. and Campins, H. (2006) Origin of Water on the Terrestrial Planets. In: Daniela, L., Sylvio Ferraz, M., Angel, F.J. (Eds.), *Asteroids, Comets, Meteors,* v. 229, IAU Symposium, p. 381-394.
- Duncan, M. J., Levison, H. F., and Lee, M. H. (1998) A Multiple Time Step Symplectic Algorithm for Integrating Close Encounters. *Astron. J.,* v. 116, p. 2067-2077.
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- O'Brien, D. P., Morbidelli, A., and Levison, H. F. (2006) Terrestrial Planet Formation with Strong Dynamical Friction. *Icarus,* v. 184, p. 39-58. doi:10.1016/j.icarus.2009.04.005
- Taylor, G. J. (November 2008) Tiny Molten Droplets, Dusty Clouds, and Planet Formation. *Planetary Science Research Discoveries.* http://www.psrd.hawaii.edu/Nov08/chondrule_sodium.html.

Other quantitative models of planetary formation:

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- Chambers, J. E. (2004) Planetary Accretion in the Inner Solar System. *Earth Planet. Sci. Lett.,* v. 223, p. 241-252.
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- Raymond, S. N., O'Brien, D. P., Morbidelli, A., and Kaib, N. A. (2009) Building the Terrestrial Planets: Constrained Accretion in the Inner Solar System. *Icarus,* v. 203, p. 644-662, doi:10.1016/j.icarus.2009.05.016.
