DESIGN OF PEBBLE-BED REACTORS USING GENETIC ALGORITHMS

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ABSTRACT: We present a conceptual design approach for high-temperature gas-cooled reactors using recirculating pebble-bed cores. The --design approach uses PEBBED, a reactor physics code specifically designed for equilibrium cycle analysis of pebble-bed reactors (PBRs), in conjunction with a *genetic algorithm* to obtain a core that maximizes a fitness value that is a function of user-specified parameters. The uniqueness of the asymptotic pattern and the small number of independent parameters that define it suggest that a PBR core and fuel cycle can be efficiently optimized given a specified objective. In this paper, candidate core geometries are evaluated primarily on the basis of core multiplication factor and peak fuel temperatures, but core radius and pumping power can be considered as well. A design that achieves the criticality and passive safety objectives can be analyzed and further optimized with more detailed and sophisticated models. Fuel management schemes involving multiple pebble types and flow zones were optimized as part of this study. The method has been successfully employed to design a Very High Temperature Reactor as part of the US Department of Energy's Next Generation Nuclear Plant program. A 600 MWt pebble bed VHTR was designed with passive safety characteristics, superior fuel economy, and resistance to steam ingress. Passive safety (peak accident temperatures < 1600 ^{o}C) was confirmed with the safety analysis code MELCOR. The INEEL's PEBBED code is the first pebble bed analysis and design tool to employ advanced optimization techniques.

0. INTRODUCTION

We present a method for the conceptual design of recirculating pebble-bed reactors, including Very High Temperature Reactors (VHTR). The design approach uses a reactor physics code specifically designed for pebble-bed reactors (PBRs) to generate core neutronic and thermal data rapidly for the asymptotic (equilibrium) core configuration. The passive safety characteristics are confirmed using a more sophisticated accident analysis code and model. The uniqueness of the asymptotic pattern and the small number of independent parameters that define it suggest that the PBR fuel cycle can be efficiently optimized given a specified objective. This is demonstrated with the application of a *genetic algorithm,*[i] a stochastic, multivariable optimization technique that searches over a large domain to find a solution that yields a best fit to specified requirements.

In this paper, the fitness of candidate core geometries is evaluated on the basis of user-specified traits such as core multiplication factor and peak accident fuel temperature. Pumping power and pressure vessel fast fluence are considered as well. A design that achieves the criticality and passive safety objectives can be analyzed and further optimized with more detailed and sophisticated models. The method has been applied to optimize an early version (268 MW_t) of the Pebble Bed Modular Reactor,[ii] a 300 MW_t PBR designed for process heat applications, and 600 MW_t VHTR. The results of the VHTR-600 are discussed herein.

1. BACKGROUND AND APPROACH

1.1 Analytical Tools

The INEEL code PEBBED[iii] is used for self-consistent analysis of neutron flux and isotopic depletion and buildup in a PBR with a flowing core. The code can treat arbitrary pebble recirculation schemes, and it permits more than one type of pebble to be specified. The key is the use of a recirculation matrix[iv] that adequately describes the flow distribution in the core in terms of a few basic core parameters so that pebble flow is tightly and efficiently linked to nuclide burnup. At the INEEL, the PEBBED code has already been applied to treat a variety of practical PBR problems such as a two-zone concept considered as a candidate for construction in South Africa. This core consists of two concentric zones with different pebble types (pure graphite and a fuel-graphite mixture). Another is the PBR version of an OUT-IN fuel cycle in which fresh pebbles are circulated in an outer annulus until an intermediate threshold burnup is attained. The partially spent pebbles are then transferred to the inner central column for the remainder of their core lives. Output from PEBBED includes the spatial distribution of the burnup and of the principal nuclides throughout the reactor core and in the discharged pebbles. The code allows estimation of refueling needs and predicts the power production.

The large number of core configurations required for a sensitivity study, or a conceptual design effort, prohibits the extensive use of sophisticated thermal-hydraulic models. Fortunately, the nature of coolant flow in a pebble-bed and the large height-to-diameter ratio allow for reasonably accurate determination of mean and peak fuel temperatures using one-dimensional models.[v,vi] Coolant flow and heat transfer correlations appropriate for pebble beds have been implemented into the code to provide estimates of the temperature distribution in the core during normal operation. A one-dimensional radial transient conduction-radiation calculation is used to *conservatively* determine the peak fuel temperature during a depressurized loss-of-flow accident. Since this study was performed, work has commenced on implementing a two-dimensional thermal-hydraulics module into PEBBED as well as thermal and leakage feedback in cross-section generation.

1.2 Genetic Algorithm Optimization

A manual search for a reactor design was conducted as part of a project to develop a pebble-bed version of the VHTR.[vii] A range of potentially promising core and reflector sizes were sampled and the results were tallied. This approach did yield a conceptual design that satisfied the requirements of the design study yet this approach is inefficient and unlikely to result in the best possible design. A much more sophisticated approach is desired. Recently, an optimization feature was added to PEBBED to perform design studies. The new tool was developed with funding from a DOE Nuclear Energy Research Initiative grant. Preliminary results of its application to the PBR are provided here. PBRs with different fuel loading patterns have been optimized using this tool and the results will be presented in future publications. The results of a search for an improved 600 MWt VHTR are presented here.

The advanced optimization component now available in PEBBED is based upon a genetic algorithm. A genetic algorithm is a stochastic search method in which a randomly generated population of test designs is analyzed. The attributes (genes) of test designs with the greatest fitness values, as specified by the user, are combined to generate a new population of presumably more fit individuals. Selection of the fittest designs, mixing or crossover of genes, and even the random mutation of genes are performed in a process that is a close analog of biological evolution with analogs of selection, gene-blending (cross-over), and mutation.

Genetic Algorithms have been used for a wide variety of optimization applications, including LWR fuel cycle optimization. The problem starts by coding the important attributes (genes) of the system either as a binary word (i.e., a series of zeros and ones) or as real numbers. A ‘net’ is cast over the domain of the solution space by randomly generating the genes for a specified number (population) of ‘individuals’. Genotypes (e.g., core attributes) that produce favorable ‘traits’ (e.g., acceptable peak fuel temperature and/or fast fluence near the pressure vessel) are passed along to the next generation. An overall fitness value is generated for each individual core design based upon a user-specified function of the traits. In a process called *selection*, a specified fraction of the population with the highest fitness values are allowed to ‘survive’ and form the gene pool for the next generation. Attributes of two randomly chosen survivors are mixed to form two new individuals in a *crossover* process that is mathematically analogous to genetic breeding. The population is thus rebuilt from the fittest individuals and the process is repeated. The selection and crossover processes alone may, however, lead to a loss in population diversity and converge to a local fitness maximum. Therefore, a third process, *mutation* is employed. This low probability event involves changing the gene of an individual to a randomly chosen new value within the variable domain. In this way, the search is directed toward previously unexplored regions of the solution space that may yield better local, and hopefully a global, optima.

Finding a global optimum nestled within a large number of local optima more than a brute force random search. In a genetic algorithm, search refinement is achieved using ‘mutation’ and ‘cross-over’ processes. In mutation, there is a small (say, 1 in 10^4) possibility that a bit in the string will be arbitrarily changed to the opposing value. This does not advance the search for a solution but it does prevent the development of a uniform population unable to ‘evolve’. Crossover refers to the exchange of genes in which the favorable parts of two parents are combined to produce an offspring that contains both.

In real-coded genetic algorithms, population characteristics are stored as real variables rather than binary words. Crossover may result in the direct transposition of genes from the parents but it also may result in a hybrid, i.e., a weighted average of the genes of the parents. A wide variety of “crossover operators” have been proposed and employed in different optimization routines.

Crossover does not guarantee that the offspring solution will be superior but it does focus the search algorithm on regions that have a higher concentration of favorable attributes. The three attributes of selection, mutation, and crossover are direct analogs of biological reproduction with recombinant DNA.

Because of the ease of use and effectiveness, genetic algorithms have been the subject of much study and broad application, including light water reactor core design.

1.2.1 Genes, Traits, and Fitness

The *fitness* of an individual (a candidate design) is a function of its traits, as specified by the user. Fitness specifications are developed for the three cases stated above, and the results of the optimization are presented. PEBBED allows the user to specify the variables (genes) over which the search is to be performed. For this design study, variables included the inner reflector radius, the fuel annulus width, the core height, and the fraction of total pebble flow that is in the outer zone (of a two-zone core). These variables were allowed to vary over a range specified in an input file containing the optimization parameters.

The user then specifies the core characteristics or *traits* that determine fitness. Currently in PEBBED, traits include equilibrium core eigenvalue, maximum D-LOFC fuel temperature, outer reflector radius, ratio of required pumping power to total thermal power, peak operating fuel temperature, maximum particle power, and reactivity.

The way in which these traits are factored into the overall fitness is with a user-specified 4-point interpolation scheme. As an example, the maximum accident fuel temperature fitness is illustrated in Figure 1.

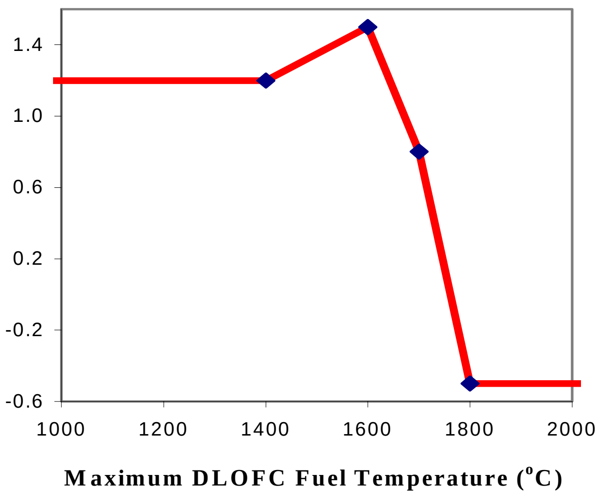

FIGURE **1***: Example of a four-point peak fuel temperature contribution to the fitness specification.*

If this trait were the only one to be specified in an optimization run, the algorithm would be driven toward a set of genes that yield a peak accident fuel temperature of 1,600°C. Above this value, the fitness value drops and even goes negative as a value of 1,800°C is approached. Negative values can be used to strongly penalize designs that exhibit completely unacceptable traits such as exceeding fuel failure temperatures during a D-LOFC transient. Figure 2 illustrates the fitness contribution from core multiplication factor used in this study.

The contributions from all selected traits are summed to yield the overall fitness of the individual. For example, core eigenvalue, maximum DLOFC fuel temperature, outer reflector radius, and height were the selected traits in the optimization of the VHTR (next section).

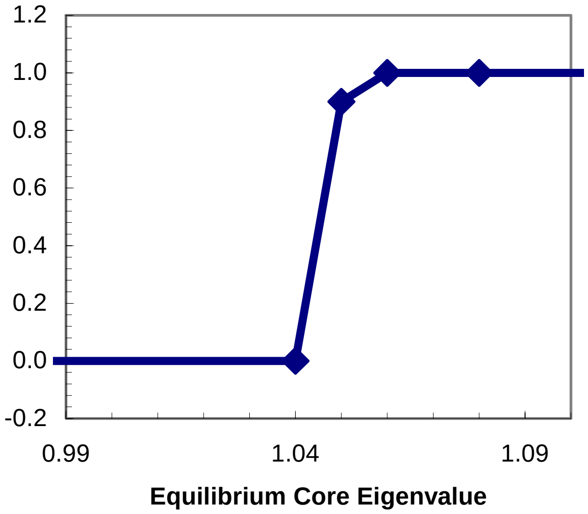

FIGURE 2*: Example of eigenvalue contribution to the fitness specification.*

The plot achieves its maximum at 1.06 (3rd point) and then is constant for higher eigenvalues. This allows for the negative reactivity of fission products not currently modeled in PEBBED and control rods that may be used to hold down any excess reactivity that is used for power manipulation. Holding it constant above that value means that cores with higher eigenvalues will be considered neither better nor worse. The algorithm may drive the solution to k_{eff} = 1.06 if reducing it helps raise the fitness contribution of another trait.

Penalizing large diameters can help to avoid impractical designs even if they are passively safe. However, the overall magnitude of this fitness contribution is less than that from the core eigenvalue and maximum DLOFC fuel temperature because (so the author assumes in this work) it is more important to make a critical, passively safe reactor than a small one.

For small modular PBRs such as the PBMR, pumping power is not significant (1-3 MW) even though it is still larger than a comparable prismatic core. Pumping power rises with the cube of the mass flow rate so that for high power pebble-bed reactors the required pumping power can be a significant fraction of the total thermal power output and can be used as a trait when designing large (>500MW) power plants.

There is a complex interplay between the variables that specify core geometry and the traits that result. Core fitness specification itself is an art that can take considerable study. A full core design involves some testing and tweaking of the fitness functions until a fully satisfactory design is obtained. However, even the early attempts discussed in the following sections show that the method is powerful and flexible.

1.2.2 Description of the Operators

As discussed in the previous section, genetic algorithms apply three operations to a set of individuals: selection, crossover, and mutation. Variations on each of these have been applied to many different problems with varying degrees of success. For this work, no effort was made to experiment with different operators, a considerable effort in itself. Rather, a set was chosen that the author judged to be adequate for the type of problem being solved. This set was successful in producing satisfactory designs in a reasonable amount of time and are discussed in this section. Future development will likely lead to more efficient algorithms.

Selection

Individuals that exhibit superior traits “survive” into the next generation. Superiority in this algorithm simply means a higher overall fitness value as described above. The user specifies *which* traits are to contribute to the fitness and how they are to be weighted. The user also specifies the number of individuals in a population as well as the number of individuals that are allowed to survive and populate the next generation. For the efforts described in the next section, a population size of 40 was chosen. Of these, the 10 individuals in a generation that displayed the highest fitness were deemed the survivors.

Cross-over

The variables available for selection as “genes” in PEBBED (inner reflector radius, fuel annulus width, outer reflector width, active core height, fraction of core pebble flow that is in the outer zone) are all real-valued and are coded as such. The crossover operation involves taking weighted averages of the genes of two parent individuals to form two new individuals. The “parents” are selected randomly from the “survivors” of the selection operation.

The weights used in determining the genes of the offspring are computed from the fitness of the selected parents according to the following formula. Let g_1 and F_1 be the values of the gene and overall fitness, respectively, of parent 1. Likewise the subscript 2 denotes the properties of parent 2. The hybrid gene computed for the first offspring, g_1’, is given by eq. 1(a) while that of the other offspring is given by eq. 1(b).

$$g_1{}' = g_1 + \frac{F_2}{F + F_{21}}\left(g_2 - g_1\right) \qquad g_1{}' = g_1 + \frac{F_1}{F + F_{21}}\left(g_2 - g_1\right)$$

Hybrid Gene 1(a) *Hybrid Gene 1(b)*

A user-specified crossover probability value determines whether the crossover operation occurs for a given gene in a match. For the cases performed in the next section, a crossover probability of 85% was used. In other words, for each gene pair processed, there was an 85% chance that the corresponding genes of the offspring were computed in this fashion, and a 15% chance that no mixing occurred. In these cases, offspring #1 took the gene of parent 1 and offspring #2 took the gene of parent 2.

This process takes place until the population is replenished to the user-specified level.

Mutation

After the new population is formed, a mutation operation may be performed on all but the fittest individual in the population. The algorithm loops through each gene of each individual (except the fittest) and generates a random number between 0 and 1 for each. If the number is less than or equal to a user-specified mutation probability, that gene is changed to a new value. The new value is itself a randomly chosen member on the interval (gene domain) specified in the input file and thus is correlated neither to the genes of the parents nor the original value of the individual.

The three operations described above are performed on each generation. The user specifies both the number of generations and the number of individuals in the population.

2. MODEL AND RESULTS

2.1. VHTR – Characteristics and Design Objectives

The Very High Temperature Reactor is one of six advanced concepts chosen by the Department of Energy for further research and development under the Generation IV program.[viii] Of the six concepts, the VHTR offers the greatest potential for economical production of hydrogen as well as electricity because of the high outlet temperature of the helium coolant (1000 °C). This outlet temperature is one of only two absolute requirements for the candidate designs in this study. The other requirement is that the VHTR be passively safe, i.e., no active safety systems or operator action are required to prevent damage to the core and subsequent release of radionuclides during design basis events. The worst such event, the depressurized loss of forced cooling (D-LOFC), also known as depressurized conduction cooldown transient, occurs when helium pressure and flow are lost. During a D-LOFC, the negative temperature reactivity shuts down the chain reaction. However, passive safety also requires that the subsequent decay heat be removed from the core by conduction and radiation before the fuel reaches failure temperatures. For TRISO-particle-based gas reactor fuel, a conservative limit on fuel temperatures is the widely accepted value of 1600 °C.

Other desirable objectives of a VHTR design may include acceptable operating peak fuel temperature (<1250 °C) and lifetime pressure vessel fluence ($<3x10^{18}$ n/cm^2). Of course, criticality is assumed. Therefore a range of acceptable core multiplication factors (k_{eff}) was identified that allows sufficient margin to offset the reactivity hold down of minor fission products not modeled in the code. In all the designs considered here, the fuel is assumed composed of 8% enriched UO_2 in coated particles embedded in a graphite matrix. Other enrichment values are possible but were not considered in this study.

In the event of ingress, the hot graphite in the core would react with air and water in exothermic reactions. This could in turn result in core damage. This is compounded by the fact that ingress may also inject positive reactivity at a rate that could result in fuel failure, before said failure could be pre-empted by the negative reactivity feedback from the subsequent temperature increase. Proper design must include an assessment of water and air ingress reactivity.

For D-LOFC calculations, the PEBBED models assumed a stainless steel core barrel, a 30 cm gas gap between the outer reflector and core barrel, a 5 cm gap between barrel and steel pressure vessel, and a 30 cm gap between the vessel and the concrete containment. A natural circulation (air) reactor cavity cooling system (RCCS) is assumed to function as designed during design basis events. This allows the use of a constant outer wall temperature boundary condition.

A parameter unique to the recirculating pebble-bed reactor is the rate at which pebbles flow through the core. During normal operation, pebbles trickle through the core and drop out of discharge tube at the bottom of the core vessel. Typically three or four pebbles are released every minute. The burnup of each pebble is measured to determine if it is to be reloaded at the top or delivered to a spent fuel container for subsequent processing to disposal. The total pebble flow rate is limited by considerations on the physical integrity of the pebbles. In addition, the speed at which pebbles flow affects the design of the burnup measurement system. For this study, pebble flow was limited to 4500 pebbles per day (about 1 every 20 seconds) for every 300 MW_t of core power to allow for adequate burnup measurement time using two parallel fuel measurement channels.[ix] This limitation on the pebble discharge rate (and consequently on in-core flow rate) can of course be relaxed to allow higher pebble throughput merely by providing a larger number of fuel measurement channels. The limitations stemming from physical considerations on the pebbles integrity would remain however.

The models used in this study did not include control elements. This is not unreasonable for normal operation of a PBR. Semi-continuous refueling allows these reactors to operate with very little excess reactivity. Excess reactivity (a few percent Δk/k) for power adjustments can be included and held down by control rods but even this is not necessary. Nominal power variations can be effected through coolant inventory- or flow-induced thermal feedback.[x] Two independent shutdown mechanisms are required to achieve cold shutdown: control rods are inserted or absorber spheres are blown into outer reflector channels. This is adequate for modular PBRs with small diameter cores. For larger units, radial leakage may not be large enough to yield sufficient rod worth for cold shutdown. However, designs for larger cores usually feature an inner cylindrical reflector of solid graphite, the primary purpose of which is to act as a heat reservoir and reduce the thermal conduction path out of the fuel. Control rods can be inserted into this inner reflector; a region of very high neutron importance. Nonetheless, during normal operation, control rods are only partially inserted into the reflector, if at all, and thus were not modeled in this study.

The lack of excess reactivity also results in a highly proliferation-resistant power plant as indicated in previous studies.[xi] Any diversion of neutrons from power production would be either prohibitively slow or easily detectable.

A significant, though limited, number of candidate designs for the 600 MW_t VHTR were analyzed using the approximate dimensions of the General Atomics GT-MHR prismatic reactor as a starting point. Fuel pebbles used the typical 6 cm outer radius but the inner fuel radius was varied to yield better neutron economy[xii].

2.2 Results

The eigenvalue fitness contribution peaks at 1.073, the value obtained for a known reference design. Control elements and minor fission products are neglected in this model so that the core eigenvalue is expected to be higher than 1.0. The contribution of the peak DLOFC temperature was lowered to 1575 ^{o}C to provide a bit of safety margin. This is a slightly more stringent specification than the 1600 ^{o}C limit employed in the manual search. The full four-point fitness specification is summarized in Table 1.

TABLE 1. Fitness Specification for the VHTR-600 Optimization

Point	k_{eff}	F_k	DCC Peak Temp. °C	F_t	Outer Reflector Radius (cm)	F_r	Pumping Power/Core Power	F_p
1	1.04	0	1400	1.2	0	0.3	0	0.3
2	1.05	0.9	1575	1.3	100	0.3	0.05	0.15
3	1.073	1.0	1700	0.5	305.5	0	0.10	0
4	1.08	1	1800	-0.5	330	0	0.15	-0.4

The 600 MWt pebble-bed VHTR obtained using a manual search and reported in reference [vii]was used as a reference point for a genetic algorithm search. This reactor contains a solid inner reflector and a simple burnup-independent recirculation scheme. The discharge burnup was kept at a nominal 80 MWd/kg$_{hm}$. A population size of 40 was chosen, from which 10 survivors were propagated to next generation.

Table 2 shows the reference gene values from the VHTR-600 designed in the previous chapter as well as the range chosen for the genetic algorithm search.

TABLE 2: Nominal values and gene domain for the VHTR-600 optimization.

Gene	Reference VHTR-600 Value	Minimum Value	Maximum Value
Inner Reflector Radius (cm)	150	1	150
Fuel Annulus Width (cm)	100	80	120
Height (cm)	950	750	1,050

Table 3 lists the results of the manual search and the one obtained using the genetic algorithm. The genetic algorithm run required 29 hours of CPU time on a Dell Precision 650 workstation.

TABLE 3: Selected results of VHTR-600 manual and automated design runs.

	VHTPBR-600 (Manual Search)	VHTPBR-600 GA search
Inner Reflector Radius (cm)	150	147.8
Fuel Annulus Radius (cm)	250	246.6
Outer Reflector Radius (cm)	326	322.6
Height (cm)	950	991.9
K_{eff}	1.073	1.073
Maximum DLOCA Fuel Temperature (°C)	1,584	1,573
Pumping Power (MW)	26	28
Maximum Operating Fuel Temperature (°C)	1,028	1,025
Peak Particle Power (W)	0.14	0.14

The genetically designed core is slightly thinner than the reference design. The accident temperature fitness specification peak of 1575 °C is slightly lower than that used for the reference design value thus resulting in a slightly narrower core annulus. This provides a shorter conduction length to the reflectors. To recapture the desired core eigenvalue, the height of the core was raised by 42 cm. The fitness benefit of achieving the target eigenvalue was somewhat offset by an increase in the required pumping power (2 MW more than the reference design).

The outer diameter of the pressure vessel is 7.45 meters, smaller than the General Atomics prismatic GT-MHR [2] by 21 cm, but the active core is two meters taller. A proper sensitivity study should be performed to find the optimal tradeoff between diameter and height. This specification could then be incorporated directly or indirectly into the fitness specification in future design efforts.

A disadvantage of a large pebble-bed, compared to a comparably-sized prismatic HTGR, is the tremendous pumping power requirement, 26-28 MW for a 600 MWt core. This requirement effectively makes the VHTR-600 a VHTR-570 and undercuts much of the advantages derived from the superior neutron economy of the pebble-bed core. One way to compensate may be to have the coolant pass radially through the bed rather than axially in a concept recently proposed by Muto and Kato[xiii]. This improvement alone may make the difference in economic viability. PEBBED's temperature correlations are not currently able to handle cross flow so this is an option that cannot yet be explored.

3. CONCLUSION

At the time this study was performed, thermal and leakage feedback was not implemented in PEBBED. Given the very large temperature rise across the core and the presence of large internal and external reflectors, the variation in microscopic cross-sections can be significant. Therefore, the results shown above should be assumed to have large error bars. Nonetheless, the search design method involving genetic algorithms and an efficient pebble-bed core simulator is well-demonstrated.

The conceptual design of a Very High Temperature Reactor is achieved using the PEBBED code enhanced with a genetic algorithm. PEBBED employs a unique method for linking the flow of pebbles to the burnup equations that fully describes the loading scheme in terms of a few core parameters. These parameters are used as independent variables (genes) in the core design search. A fitness function, specified by the user and based upon a four-point interpolation scheme, allows the user to select and weight the core characteristics of interest. Thus, basic core design of pebble-bed reactors, even with multiple pebble types and complex flow patterns, can be automated and executed on a desktop computer.

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