

# Assessing Life Cycle Environmental Implications of Polymer Nanocomposites

This work presents the most comprehensive Life Cycle Energy Analysis of Carbon Nanofiber (CNF) based Polymer Nanocomposites (PNCs). The use of polymer nanocomposites in automotive body panels as a substitute for traditional materials is evaluated and compared with traditional materials. PNCs have enhanced mechanical properties, high strength-to-weight ratios, and are capable of offering specific functionalities such as desired level of electrical conductivity. These combinations of properties are making PNCs one of the fastest-growing materials in the plastic segment and an attractive alternative to conventional materials like steel and aluminum.

## Polymer Nanocomposites- Results and Discussion

In this study, a “cradle-to-gate” life cycle study of CNF-based PNCs is carried out. Previous work on the CNF life cycle by the authors served as a basis for this analysis. The boundaries of the CNF life cycle are expanded to include the production of PNC and the manufacture of the end product. A typical life cycle for nanocomposites is depicted in Figure 1. Alternatives exist at each processing stage for the above mentioned production methods based on the choice of feedstock and the final product manufacture. Life cycle data is compiled with information reported by the open literature. Polypropylene-based CNF nanocomposites are considered as the example. Once the CNFs are dispersed in the polymer, these reinforced materials can be either extruded or injection-molded to obtain a variety of end products.

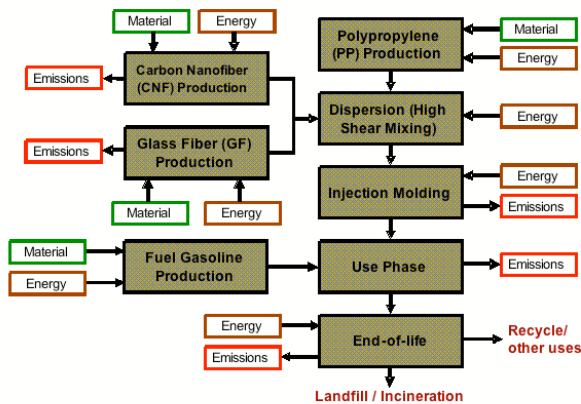


Figure 1. Typical Life Cycle of Polymer Nanocomposites

A “cradle-to-gate” energetic life cycle assessment of CNF-reinforced polypropylene is performed and compared with steel. The functional unit for comparison is the equal stiffness of different components. Five different cases are investigated with varying loading ratios of the CNF in the polypropylene matrix. Two cases with both CNFs and glass fibers are also studied. As depicted in Figure 2, it is observed that for equal stiffness of the components, on a cradle-to-gate basis, CNF-reinforced polypropylene composites are 2-

10 times more energy intensive compared with steel. It is further concluded that the product use phase might govern whether the high upstream energy can be offset during the use phase to realize any life cycle energy savings.

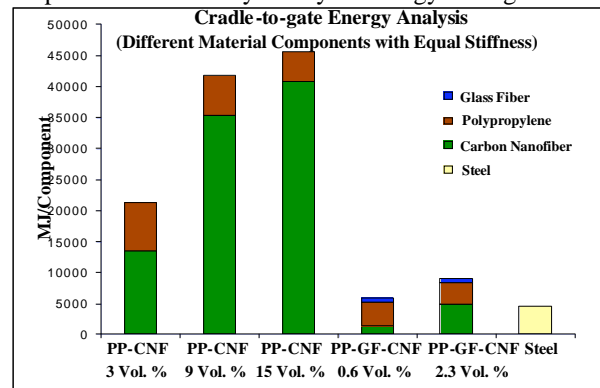


Figure 2. Life Cycle Comparison of Materials with Equal Stiffness

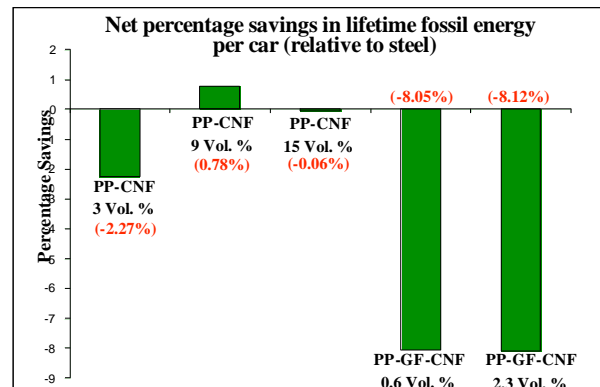


Figure 3. Polymer Nanocomposites - Application to Automotive Body Panels

Finally the use of CNF-reinforced nanocomposites in body panels of light-duty vehicles is evaluated. The life cycle of a midsize automobile with CNF-reinforced nanocomposite body panels is evaluated and compared, relative to conventional steel panels. The results are shown in Figure 3. It is concluded that the use of polymer nanocomposites in automotive body panels results in marginal life cycle energy savings. Besides, polymer-nanocomposites-based body panels with higher CNF loading ratios appear to be almost at par with steel on a total life cycle basis and do not offer any additional life cycle energy savings. Further, use of CNFs with other additives like glass fibers might be more promising for automotive applications in the near term, with net energy savings of around 8 percent relative to steel.

The results obtained have a high degree of uncertainty, owing to several reasons. Some of these are: huge life cycle energy requirements for the production of CNFs, possible achievable weight reductions of polymer-nanocomposite-based components, and the end-of-life issues specific to polymer nanocomposites that can be significant. Besides, PNCs might be difficult to recycle,

reuse, and/or dispose of compared with conventional materials like steel and aluminum. Current work is in progress to address these issues and evaluate other thermoset-based nanocomposite materials. Proxy indicators are also being explored to gain insight into the broader ecotoxicity of these engineered nanomaterials in the absence of detailed ecotoxicological studies.

## Publications

1. Vikas Khanna, Bhavik R. Bakshi, and L. James Lee, "Energy Consumption and Environmental Impact from the Life Cycle of Carbon Nanofibers", *Journal of Industrial Ecology*, accepted.
2. Vikas Khanna, Bhavik R. Bakshi, and L. James Lee, "Assessing Life Cycle Environmental Implications of Polymer Nanocomposites", (in preparation)

## Energetic and Environmental Evaluation of Titanium Dioxide Nanoparticles

Typical rutile phase pigment grade  $\text{TiO}_2$  particles are on the order of 250 nm to 1  $\mu\text{m}$  in diameter. However, recent demand for smaller particles for use in sunscreens and for catalytic applications has opened up a market for 20-50 nm anatase phase particles. The Altair hydrochloride process uses a spray hydrolysis step, which allows for further flexibility in the phase and size distribution of the produced particles. Also, an almost complete recycle of the hydrochloric acid used in the process affords energetic and monetary advantages over the older processes. The Altair hydrochloride process is shown in Figure 4.

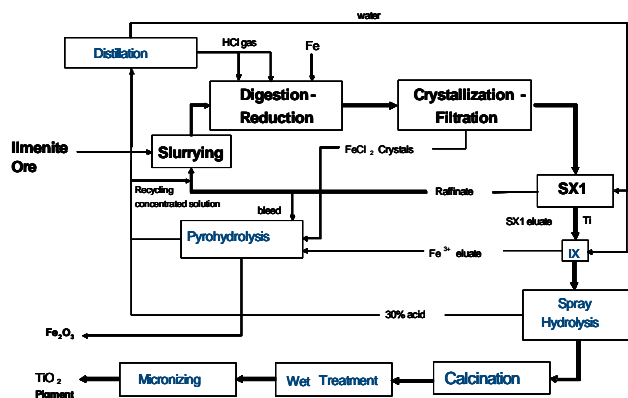


Figure 4. Process flow for Altair hydrochloride process

The current project uses the best available information to investigate energy and exergy use in the Altair  $\text{TiO}_2$  hydrochloride process at both the process and life cycle scales. The goal of this part of the project is to identify key steps that consume the most exergy and identify opportunities for improvement at both the process and life cycle scales.

## $\text{TiO}_2$ Nanoparticles- Results and Discussion

The Altair  $\text{TiO}_2$  hydrochloride process was broken into nine main process units and about 25 major flows. Energy input to each unit was calculated from process

information available in the literature from Altair. Any missing energy inputs were estimated from these publications or from other sources considering similar units. The compositions and physicochemical properties of the major flows were also taken from these publications or estimated when necessary.

The major energy inputs to the process were in the form of electricity to several units, methane to the two hydrolysis units, and high-pressure steam for the distillation unit. Overall it was found that approximately 61 MJ were required for the production of 1 kg of the final product at the process scale. This number is comparable with the findings of Reck and Richards using the older sulphate process to produce  $\text{TiO}_2$  from ilmenite. They reported values ranging from 70-80 MJ per kg of  $\text{TiO}_2$  produced.

Because the Altair hydrochloride process is a materials process, exergy analysis is especially informative because it is able to quantify the usable energy of both material and energy flows in a common unit (kJ/mol). The exergy of the major flows was calculated as the sum of the chemical and physical exergy. Potential, kinetic, and nuclear exergy were assumed to be negligible for this process.

Exergetic efficiency has been calculated for each major unit in the process. Preliminary results of this analysis show that exergy destruction is greatest in the two hydrolysis units and the distillation unit, while the exergetic efficiency is the lowest for those same units.

In order to calculate the minimum exergy required to produce one mole of  $\text{TiO}_2$  particles using this process, the inputs were scaled according to the stoichiometrically required amount of ilmenite ore to produce a single mole of product. That is to say that, theoretically, none of the titanium was lost in the process, and all avoidable exergy losses were avoided. This value was calculated to be approximately 4 MJ/mol of product.